

Spherically Symmetric Approximation (and beyond)

in

Relativistic Schrödinger Theory

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Abstract

The energy eigenvalue problem of non-relativistic positronium is considered within the framework of Relativistic Schrödinger Theory (RST), and the results are compared to those of the conventional quantum theory. For the range of principal quantum numbers $n = 2, 3, \dots, 30$, the RST predictions for the non-relativistic positronium energies deviate now from the corresponding predictions of the conventional quantum theory at an average of (roughly) 3%. These results suggest that the deviations will be further diminished in the higher orders of approximation.

The emphasis aims at the role played by the assumption of *spherical symmetry* of the gauge potential. A new approximation procedure is established in order to regard also the *anisotropic* character of the interaction potential. This reduces the deviations of the RST predictions from the corresponding conventional results by 50 percent, whereas the spherically symmetric corrections of higher order do amount only to (roughly) 0,2%. Therefore further improvements of the RST predictions may be expected by considering more rigorously the *anisotropy* of both the interaction potential and of the wave functions. Such an analysis (however complicated it may

be) seems inevitable in order to decide whether perhaps the exact RST predictions do practically coincide with those of the conventional quantum theory.

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I Introduction and Survey of Results

The present paper studies the numerical influence of the *anisotropy* of the electron-positron interaction potential on the energy spectrum of non-relativistic positronium. In some preceding papers it has been found that (even up to very highly excited states) the corresponding RST predictions come close to their conventional counterparts up to some 10 percent, already by very rough approximation methods being based on the complete neglection of the anisotropy of the interaction force. And therefore one wishes to know now whether perhaps this unexpected agreement with the conventional predictions becomes still better through including the anisotropy effect. Naturally, the physical relevance of *Relativistic Schrödinger Theory* is to be tested via the experimental verification of its numerical predictions in the various fields of possible applications (e.g. the presently considered positronium system). Concerning this specific case of demonstration, one is tempted to suppose that the *exact* RST predictions could perhaps agree (nearly or exactly) with the corresponding predictions of the conventional quantum theory. If such a result (i.e. the numerical equivalence of RST and conventional predictions) could be shown to hold for the whole field of atomic and molecular physics, this would then imply a partial dethronement of the conventional quantum mechanics. But since the latter is rather of probabilistic nature whereas RST is essentially a fluid-dynamic theory, it seems adequate and desirable to first clarify the philosophical difference of both quantum approaches, where Bohr's *complementarity principle* plays a dominant role.

1. Particle-Wave Duality and Complementarity

In the literature, one frequently encounters the viewpoint that the conventional quantum theory represents a logically perfect system which cannot be further improved by "small" modifications, neither concerning the formalism nor its predictive power. Such arrogant judgment arose early during the development of quantum theory when Born and

Heisenberg maintained 80 years ago that " *quantum mechanics is a complete theory; its basic physical and mathematical hypotheses are not further susceptible of modifications*" [1,2].

It seems that this viewpoint represents nowadays the general conviction of the community; however it seems to us that some criticism is well-suited here. Firstly, even if presently nobody is able to imagine how further improvements of the conventional theory could look like, one cannot be sure that future workers in this field will not invent more efficient logical systems which on the one hand do include their Born-Heisenberg precursor, but on the other hand do also considerably exceed it. And secondly, the present-day form of the conventional quantum mechanics as the offspring of the Born-Heisenberg construction may admittedly represent a closed logical system but it nevertheless could perhaps miss certain features of quantum matter which on principle cannot be grasped by *any* logical system of the *probabilistic* type! If this latter supposition should be true, these additional features (inaccessible to the purely probabilistic world view) would then be well-hidden behind the statistical predictions of the conventional theory.

Concerning now a possible signal for the presence of such an additional structure beyond the purely probabilistic approach, one could perhaps think of the wave-like behavior of quantum matter; and this would suggest that for the description of certain (but surely not all) quantum phenomena a fluid-dynamic approach would be better suited than the conventional probabilistic viewpoint. This *particle-wave duality* of microscopic matter has ever been thought to be the origin of those strange quantum effects which formerly did not only bother the fathers of quantum theory[3] but even nowadays do appear as a "mystery" for most of the workers in this field[4,5]. Indeed, despite the widely celebrated concept of *quantum logic*, one nevertheless likes to discuss many quantum interference effects in the classical terms of *optical imagery* [4]. Naturally, such a dichotomic (or sometimes even contradictory) view on the quantum world must have provoked attempts which try to erect some unifying framework embracing *simultaneously* both the fluid-dynamic *and* the probabilistic aspects of quantum mechanics. However, it seems that nobody was (or is)

able to construct such a unified quantum formalism; and therefore most physicists seem to accept now Bohr's original idea of complementarity[2,6]. Or, summarizing this in the words of Omnes[7]: the wave logic and the particle logic could not be united to a larger consistent logic which contains both of them as sublogics and consequently, according to Omnes[7], we have to learn to live with two mutually excluding logics and nevertheless can have a true theory!

It seems that Bohr[6] was the first who grasped this logical dilemma to its full extent by establishing his "*principle of complementarity*", whereas others weakened or misinterpreted (or even misunderstood) this original idea of Bohr (for a historical account see ref. [8]). For instance, Pauli "*in his article for the Handbuch der Physik [9] called two classical concepts - and not two modes of description - complementary, if the applicability of the one (e.g., position coordinate) stands in relation of exclusion to that of the other (e.g., momentum) in the sense that any experimental setup for measuring the one interferes destructively with any experimental setup for measuring the other. Pauli, as we see, in contrast to Bohr, ascribed complementarity to two notions which belong to the same classical mode of description (e.g., the particle picture) and not to two mutually exclusive descriptions*"(ref.[2], p. 369).

An other example of distortion of Bohr's complementarity proposal is given by C.F. von Weizsäcker who said "*The complementarity between space-time description and the claim of causality is therefore precisely the complementarity between the description of nature in classical notions and in terms of the ψ function*" (ref.[2], p.369). Thus, von Weizsäcker in contrast to Pauli, interpretes correctly Bohr's complementarity principle, namely as referring to two mutually excluding "modes of description" (or "logics", as Omnes terms it [7]); but in contrast to Bohr, von Weizsäcker obviously thinks that these two (mutually excluding) modes should refer to the classical and the quantum-mechanical description of nature.

However, concerning that notorious concept of *complementarity*, we do neither join

here to the misunderstanding of Pauli nor to that of v. Weizsäcker; but rather we cling to Bohr's original idea which says that the notion of complementarity must refer to two mutually excluding logical systems (or "pictures") which both are to be used for the description of *quantum* (!) systems, i.e. the *probabilistic* point-particle picture in opposition to the *fluid-dynamic* wave picture of the elementary matter. If Bohr's complementarity principle is understood in this way (i.e. more precisely: is understood in the sense of Omnes[7]), the logically coherent and causal space-time descriptions of classical particles and waves (e.g. "Classical Electrodynamics" [10]) must be broken up for the transition to the quantum-mechanical description into two mutually excluding modes of description (or "logics") for the massive particles, namely into the probabilistic point-particle picture with its lack of a physical mechanism for the local but "indeterministic" collapse of the probability distribution and into the fluid-dynamic wave picture with its inability to predict the instantaneous statistical correlations between widely separated regions of three-space (see the EPR phenomena [4,5]). This particle-wave duality is in the first line thought to refer to the quantum mechanics of the classical massive particles, whereas the classical massless fields are left untouched in the first step of quantization. In this context, one could perhaps mention in favour of RST that this theory provides a *dynamical* mechanism for the (otherwise only *kinematically* describable) exchange phenomena! These are brought forth by the exchange potential \mathcal{B}_μ as that part of the bundle connection \mathcal{A}_μ which is responsible for the non-Abelian character of the theory.

Thus, each of the two mutually exclusive *quantum* fragments (i.e. probabilistic particle vs. fluid-dynamic wave picture), being left behind from the classical causal space-time description, suffers from a certain deficiency if viewed from the side of the original classical approach. And consequently one will hesitate to attribute to one or the other of the two competing quantum approaches the status of *completeness* (being mostly claimed in favour of the probabilistic particle picture alone, i.e. the "conventional quantum theory" [1]).

2. Relativistic Schrödinger Theory

Accepting now the necessity of two mutually excluding logical systems (albeit only as the preliminary state of the art), one might think that these two pictures have been elaborated in a comparably symmetric manner during the past development of quantum theory. However, it seems to us that just the contrary did occur: the generally accepted and almost exclusively applied form of quantum theory is based upon the probabilistic particle picture (i.e. the "conventional quantum theory"), whereas a fluid-dynamic description of quantum matter has not been tried at all, apart from a few isolated (but in the meantime forgotten) attempts. Such a situation may now be taken as sufficient motivation in order to establish a fresh fluid-dynamic approach to quantum matter which is able to counterbalance the conventional probabilistic particle logic, from both the mathematical and physical point of view. As such a competitor of the fluid-dynamic type, there has recently been proposed the *Relativistic Schrödinger Theory* (RST), see the precedent paper [11] and the other papers cited therein. Indeed, this fluid-dynamic theory differs from its probabilistic competitor (i.e. the conventional probabilistic theory) in both the mathematical and physical respect: **(i)** the many-particle systems are described in RST by the Whitney sum of one-particle fibre bundles, not by the tensor product of one-particle Hilbert spaces (as in the conventional theory); and **(ii)** the RST wave functions ψ (as the sections of complex vector or spinor bundles) are used in order to construct *physical densities* of charge, current, energy-momentum etc., not in order to construct probabilities as in the conventional theory!

However, the essential point with such two mutually excluding competitors is now that they both are expected to describe the same quantum world; and therefore there must exist certain intersecting domains of application for which both proposals make definite predictions. Clearly, if both theoretical frameworks should pretend to the same physical relevance, they are required to produce identical numerical predictions in that intersecting domain of applications.

3. Test Case: Non-Relativistic Positronium

One such common field of competition certainly refers to the energy (E) of bound systems. This physical quantity emerges in the probabilistic particle picture as the eigenvalue of the Hamiltonian \hat{H} of the considered system

$$\hat{H}\psi = E\psi . \quad (\text{I.1})$$

On the other hand, the fluid-dynamic character of RST lets emerge the total energy E_T of any RST field configuration as the spatial integral of the total energy density ${}^{(T)}T_{00}(r)$

$$E_T = \int d^3\vec{r} {}^{(T)}T_{00}(\vec{r}) \quad (\text{I.2})$$

where the energy density ${}^{(T)}T_{00}(r)$ is the time-component of the total energy-momentum density ${}^{(T)}T_{\mu\nu}$. Now it has already been demonstrated explicitly for the (relativistic and non-relativistic) hydrogen atom that the particle-like energy E (I.1) is numerically identical to the fluid-dynamic RST energy E_T (I.2); and this identity holds for all bound *one-particle* systems [12].

Therefore the desired comparison of the RST and conventional predictions must refer to the *many-particle* systems which receive a quite different treatment by each of both theoretical frameworks. Perhaps the simplest one of this non-trivial class of test cases is the non-relativistic positronium system which consists of two oppositely charged Dirac particles of the same rest mass M . The corresponding (non-relativistic) Hamiltonian \hat{H} (I.1) of this two-body arrangement reads

$$\hat{H} = \frac{p_e^2}{2m} + \frac{p_p^2}{2M} - \frac{e^2}{|\vec{r}_e - \vec{r}_p|} , \quad (\text{I.3})$$

and the conventional Schrödinger equation (I.1) of this two-body problem can be separated into the center-of-mass motion and the relative motion of the electron and positron (see any standard textbook about quantum mechanics, e.g. ref. [13]). The conventional energy spectrum of the relative motion is essentially the same as for the ordinary hydrogen

problem (with infinitely heavy proton) where merely the mass M of the electron must be replaced by the reduced mass $M/2$; i.e. the conventional non-relativistic energy spectrum of positronium is given by

$$E_{\text{conv}}^{(n_c)} = -\frac{e^2}{4a_B} \cdot \frac{1}{n_c^2} \simeq -\frac{6,8029\dots}{n_c^2} [\text{eV}] \quad (\text{I.4})$$

$$\left(a_B = \frac{\hbar^2}{Me^2} \dots \text{Bohr radius} \right)$$

where $n_c = 1, 2, 3, 4, 5 \dots$ is the principal quantum number of the conventional theory. On the other hand, a first tentative RST calculation on the basis of a two-parameter trial amplitude has reproduced this conventional spectrum (I.4) up to some few percents of deviation [12, 14]. Thus, a first crucial test for the physical relevance of the RST predictions may be referred to the accuracy of the reproduction of the conventional spectrum (I.4) when better approximation techniques are applied in RST; and this is just the main goal of the present paper.

However, as will readily become evident, the RST treatment of positronium is much more complicated than is its counterpart in the conventional theory, even in the non-relativistic domain. But this complication is not an intrinsic feature of RST but is rather a consequence of the (purely technical) fact that exact solutions of the RST eigenvalue problem are very hard (or even impossible) to obtain. The RST eigenvalue problem itself is a simple matter from the purely conceptual viewpoint since it consists merely in a simple (albeit coupled) system of two equations, i.e. the Schrödinger-like equation (III.34) and the Poisson equation (III.36). But despite its structural simplicity, this system needs considerable work in order to construct approximate solutions (see below). In contrast to this, the conventional eigenvalue problem (I.1) plus (I.3) admits exact solutions which can easily be worked out because the internal (i.e. relative) motion agrees with the standard hydrogen problem whose solutions can be read in any textbook of elementary quantum mechanics. But in view of such a fortunate situation with the conventional theory, one should not forget the fact that the conventional eigenvalue problem (I.1) plus

(I.3) cannot be deduced from a generally valid *relativistic quantum mechanics* for many-particle systems (not to be confused with quantum field theory!). It is true, the well-known Bethe-Salpeter equations are intended to represent such a relativistic quantum mechanics for many-particle systems, but they seem to be afflicted by many deficiencies and are therefore not generally accepted [15, 16]. Presumably, these deficiencies in the relativistic domain must necessarily emerge as a consequence of the probabilistic nature of those equations.

On the other hand, RST provides a consistent logical framework for relativistic N-particle systems where the particles interact via the principle of minimal coupling which then identifies RST as a relativistic gauge field theory (being Abelian for different particles and Non-Abelian for identical particles). Within such a framework, one can easily deduce a well-defined non-relativistic limit of the relativistic wave equations but the corresponding non-relativistic interaction potential depends now on the quantum state of the two-body system (in contrast to the state-independent Coulomb potential (I.3)); and additionally the interaction potential is now also anisotropic (in contrast to the spherical symmetry of the conventional Coulomb potential (I.3)). This entails that we have to solve *simultaneously both* the wave equations for the material particles *and* the gauge field equations for the interaction potentials! As a consequence, such simple exact solutions as for the conventional Coulomb problem (I.1)-(1.3) are not available for the RST case; and therefore one has to put much effort in the development of appropriate approximation techniques. This will require a large part of the paper.

4. Spherically Symmetric Approximation

But here we can resort to the fact that the coupled matter and gauge field equations may be obtained by extremalizing the RST energy functional $\tilde{E}_{[T]}$, both in the relativistic and non-relativistic situations. This provides us with the possibility to invent trial configurations with a certain number of variational parameters whose values become then fixed

through extremalization of the corresponding value of the energy functional $\tilde{E}_{[T]}$ on just those trial configurations. Moreover, this method allows us to try spherically symmetric configurations in order to avoid the necessity to deal with anisotropic interaction potentials. Of course, one might suppose here that such a spherically symmetric approximation could eventually produce unacceptable large deviations from the true RST result. But amazingly enough, the contrary seems to be true: by use of hydrogen-like trial amplitudes of $SO(3)$ symmetry one gets already in lowest approximation order RST predictions for the non-relativistic positronium spectrum, which come close to the conventional prediction (I.4) up to 10% or less [11, 14], even for the highly excited states.

From these tentative results we conclude that the RST predictions could eventually come still closer to their conventional counterparts if one would admit anisotropic trial configurations and would also apply trial amplitudes with a larger number of variational parameters. Thus, there naturally arises the question which of both effects is the dominant one: Is it more effective to improve the spherically symmetric approximation by resorting to trial amplitudes with more than two variational parameters; or is it more promising to take into account the anisotropy of the interaction potential? Or are both effects of the same order of magnitude?

The answer will turn out in favour of the anisotropic corrections which do diminish the RST deviations up to 50%; whereas the higher-order corrections of the spherically symmetric type amount to merely 0,2%.

These results are worked out now in the following arrangement:

A. RST Fundamentals

In **Sect.II**, the RST fundamentals are briefly presented to that extent which is necessary for the subsequent discussion of the positronium level system. Here the point of departure is the coupled system of matter equations (II.1) and gauge field equations (II.20).

By splitting off the usual exponential time-factor from the Dirac four-spinors $\psi_a(\vec{r}, t)$, cf. (II.10), one gets the *mass eigenvalue equations* which are written here in Pauli form, i.e. in terms of 2-spinors $\varphi_{\pm}(\vec{r})$, see equation (II.17) below. The corresponding time-independent form of the gauge field equations turns out as the ordinary Poisson equation for the electrostatic interaction potential ${}^{(p)}A_0(\vec{r})$, see equation (II.27) below. Thus the combination of the mass eigenvalue equation (II.17) and the Poisson equation (II.27) just represents the RST eigenvalue problem for positronium.

At this stage, the eigenvalue system is still fully relativistic with the *mass eigenvalue* M_* to be determined in one step together with the Pauli eigenspinors ${}^{(p)}\varphi_{\pm}(\vec{r})$ and the gauge potential ${}^{(p)}A_0(\vec{r})$. However, these positronium eigenvalue equations do not represent the most general situation, for (i) the magnetic effects are neglected (\rightsquigarrow *electrostatic approximation*) and (ii) the *exchange interactions* are also omitted since this kind of force can be active only for *identical* particles. Of course, this absence of the magnetic and exchange interactions does considerably simplify the eigenvalue problem which, however, is still left too complicated in order that exact solutions could be found.

B. Spherical Symmetry

But fortunately, there does exist an energy functional $\tilde{E}_{[T]}$ (II.32) whose extremal equations do just coincide with those coupled mass eigenvalue and gauge field equations which define the RST eigenvalue problem. The corresponding variational principle (II.40) is the *RST principle of minimal energy* which can now in **Sect.III** be exploited for obtaining approximate solutions for the considered positronium eigenvalue problem (\rightsquigarrow *spherically symmetric approximation*). This approximation method works as follows:

In order to explicitly solve the mass eigenvalue equations one has in any case to parameterize the Pauli spinors by means of both the spinor basis and the associated spinor components. The RST hypothesis for this parameterization procedure is now that

the fermionic or bosonic character of the bound system as a whole is present already in any of its constituents. Since positronium (as a whole) is a boson, both constituents (electron and positron) do therefore also adopt bosonic character, i.e. the constituent Dirac four-spinors must be decomposed with respect to a *bosonic* spinor basis which then turns out to be double-valued, see equation (III.5) below.

But once the desired decomposition of the Pauli spinors ${}^{(p)}\varphi_{\pm}(\vec{r})$ into its components ${}^{(p)}\mathcal{R}_{\pm}$, ${}^{(p)}\mathcal{S}_{\pm}$ (i.e. the “wave amplitudes”) has been attained, see equations (III.9a)-(III.9b) below, then one can write down the eigenvalue equations in terms of these wave amplitudes, (III.15a)-(III.16). This set of equations is now the point of departure for separating off the angular part of the wave amplitudes; however, this separation process can be performed *exactly* only if the electrostatic gauge potential ${}^{(p)}A_0(\vec{r})$ is *spherically symmetric*. But on the other hand, this symmetry for the gauge potential can not be exactly realized, if the angular separation process for the wave amplitudes is required to be exactly feasible, as described by equations (III.17a)-(III.17b) below. The reason for this is that the gauge potential ${}^{(p)}A_0(\vec{r})$ must be anisotropic in any case even if the wave amplitudes are adopted to exactly obey the spherical symmetry, see the Poisson equation (III.16). Therefore we have to put in by hand the *spherically symmetric approximation* which consists just in the postulate that the interaction potential ${}^{(p)}A_0(\vec{r})$ (but not the wave amplitudes themselves) be spherically symmetric, see equation (III.1) below. But once this approximation assumption is accepted, it becomes a rather straightforward procedure to get the desired approximate energy spectrum (for the present purpose we are satisfied with the non-relativistic situation). Namely, after the selection of a nearby trial amplitude $\tilde{\Phi}(r)$ (see equation (III.50) below) and computation of the associated gauge potential ${}^{(p)}A_0(\vec{r})$ (**App.A**) one substitutes this trial configuration $\{\tilde{\Phi}(r), {}^{(p)}A_0(\vec{r})\}$ into the non-relativistic energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) and then one minimizes the resulting energy function $\mathbb{E}^{[IV]}(\beta, \nu)$ (III.55) with respect to the two variational parameters β and ν which are contained in the chosen trial amplitude $\tilde{\Phi}(r)$.

This minimalization process yields then the energy spectrum displayed in **table 1** on p. 44, from where it is obvious that these RST predictions for the positronium energy levels deviate from the conventional predictions E_{conv} (I.4) mostly by less than 10%. Indeed, this is a somewhat amazing result in view of such a simple trial amplitude $\tilde{\Phi}(r)$ (III.50) with only two variational parameters. Moreover, the deviation from the conventional predictions E_{conv} decreases with increasing principal quantum number n_c , so that for high quantum numbers $n_c \lesssim 100$ one arrives at deviations by less than 4%, see **table 1** on page 44.

Clearly, such a result must evoke now some urgent questions:

- i) Is that RST deviation of some few percent an *intrinsic* feature of RST (and therefore not improvable); or is it merely due to the applied approximation method? In the latter case, the *exact* RST predictions could possibly coincide with their conventional counterparts (I.4).
- ii) If the deviation is due to the approximation method, is this deviation then an inevitable consequence of the use of the spherically symmetric approximation or is it merely due to the selection of a very rough trial amplitude $\tilde{\Phi}(r)$ (III.50) with too few variational parameters? In the latter case it would be worth while to try $O(3)$ symmetric functions with more than two variational parameters.
- iii) If the deviation is due to the use of spherically symmetric trial configurations, can then the RST predictions be improved by resorting to *anisotropic* gauge potentials?

These questions will receive the following answers by the subsequent elaborations:

- (i) the former 10% deviations [11] from the conventional results (I.4) can be pressed down to roughly 3% by resorting to the higher orders of the chosen approximation method. This supports the expectation that even higher orders of approximation will shift the RST predictions further towards their conventional counterparts (I.4).

- (ii) the RST predictions do receive an improvement of merely 0,2% if the trial configurations are restricted to obey the spherical symmetry
- (iii) The reduction of the deviations from (roughly) 10% to 3% is due to the use of *anisotropic* interaction potentials which therefore provide the possibility for even further improvements.

II RST Eigenvalue Problem

From a more philosophical viewpoint, the subsequent relativistic mass eigenvalue problem is to be conceived as the RST counterpart of the non-relativistic Schrödinger energy eigenvalue problem, i.e. the eigenvalue problem of the Hamiltonian \hat{H} . The latter problem appears as the time-independent specialization of the general time-dependent Schrödinger equation when a certain factorization ansatz for the wave function is adopted so that the usual exponential time factor can be splitted off. The solutions of the remaining time-independent equation describe then the groundstate and the excited states of the considered bound system. The same logical arrangement does apply also to the corresponding RST eigenvalue problem where, however, the gauge field equations for the interaction potentials of the material particles must complete the matter wave equations! It should be obvious that such a highly interactive system will necessitate to solve simultaneously for *both* the matter fields *and* the interaction potentials. Since exact solutions of such an intricate system are very difficult to obtain we resort to an approximation method. This consists in adopting some physically plausible trial function which contains a certain set of variational parameters serving for extremalizing the RST energy functional. Indeed, the extremal equations of that energy functional are identical to the system of coupled matter and gauge field equations forming the RST eigenvalue problem.

Obviously this program requires to discuss the following items in due order: **(i)** wave equations for the matter subsystem, **(ii)** equations for the gauge field subsystem, **(iii)** stationary bound systems, **(iv)** energy functional and principle of minimal energy, and **(v)** spherically symmetric vs. non-symmetric trial functions.

1. Matter Subsystem

Quite generally, the dynamics of the spinning quantum matter is described in RST by the N-particle Dirac equation

$$i\hbar c \mathbb{I} \Gamma^\mu \mathcal{D}_\mu \Psi = \mathcal{M} c^2 \Psi . \quad (\text{II.1})$$

Here, for the considered two-particle system (i.e. positronium), the two-particle *velocity operator* \mathbb{I}_μ is the direct sum of the ordinary Dirac matrices γ_μ

$$\mathbb{I}_\mu = (-\gamma_\mu) \oplus \gamma_\mu \quad (\text{II.2})$$

where the minus sign refers (by convention) to the “first” particle (i.e. the positron). Furthermore, the two-particle wave function Ψ is adopted in RST to be the *Whitney sum* of the two one-particle wave functions ψ_a ($a = 1, 2$)

$$\Psi(\vec{r}, t) = \psi_1(\vec{r}, t) \oplus \psi_2(\vec{r}, t) \quad (\text{II.3})$$

which says that each of the two particles does occupy a well-defined one-particle quantum state.

The gauge-covariant derivative (\mathcal{D}) emerging in the basic equation (II.1) is defined as usual in the gauge theories, i.e.

$$\mathcal{D}_\mu \Psi = \partial_\mu \Psi + \mathcal{A}_\mu \Psi , \quad (\text{II.4})$$

where the gauge potential \mathcal{A}_μ takes here its value in the Lie algebra of the *structure group* U(2) and may therefore be decomposed as follows

$$\mathcal{A}_\mu = \sum_{a=1}^2 A^a{}_\mu \tau_a + B_\mu \chi - \overset{*}{B}_\mu \bar{\chi} . \quad (\text{II.5})$$

Strictly speaking, this general form of the gauge potential does apply for a system of *identical* particles which are subjected to the *exchange forces* (being described by the

exchange potential B_μ). But since the presently considered positronium system consists of two *different* particles (i.e. positron and electron), the exchange potentials B_μ, \bar{B}_μ^* as the components of \mathcal{A}_μ with respect to the *exchange generators* $\chi, \bar{\chi}$ must vanish ($B_\mu \equiv 0$). Thus we are left alone with the purely electromagnetic interactions which are described by the electromagnetic potentials A^a_μ ($a = 1, 2$) as the components of \mathcal{A}_μ with respect to the *electromagnetic generators* τ_a :

$$\mathcal{A}_\mu \Rightarrow \sum_{a=1}^2 A^a_\mu \tau_a = {}^{(1)}A_\mu \cdot \tau_1 + {}^{(2)}A_\mu \cdot \tau_2 . \quad (\text{II.6})$$

And finally, the *mass operator* \mathcal{M} in equation (II.1) can be taken to be proportional to unity (1) for the present situation where both particles have the same rest mass (M , say)

$$\mathcal{M} = M \cdot \mathbf{1} . \quad (\text{II.7})$$

In order to further proceed towards the time-independent eigenvalue equations, one first decomposes the original two-particle equation (II.1) into two one-particle equations for the one-particle wave functions $\psi_1(\vec{r}, t)$ and $\psi_2(\vec{r}, t)$:

$$i\hbar c \gamma^\mu D_\mu \psi_1 = -Mc^2 \psi_1 \quad (\text{II.8a})$$

$$i\hbar c \gamma^\mu D_\mu \psi_2 = Mc^2 \psi_2 . \quad (\text{II.8b})$$

Here, the gauge-covariant derivative (D) for each wave function ψ_a ($a = 1, 2$) is defined as follows:

$$D_\mu \psi_1 = \partial_\mu \psi_1 - i {}^{(2)}A_\mu \cdot \psi_1 \quad (\text{II.9a})$$

$$D_\mu \psi_2 = \partial_\mu \psi_2 - i {}^{(1)}A_\mu \cdot \psi_2 \quad (\text{II.9b})$$

which expresses the fact that the two different positronium constituents are not able to feel the exchange forces ($\rightsquigarrow B_\mu \equiv 0$) but are subjected exclusively to the electromagnetic interactions!

Next, one has to face the problem of time-dependence of both wave functions $\psi_a(\vec{r}, t)$ where one naturally will expect that the relevant physical objects must be time-independent

for a stationary bound system. In this sense, one tries the usual factorizing ansatz for the one-particle wave functions $\psi_a(\vec{r}, t)$ ($a = 1, 2$)

$$\psi_a(\vec{r}, t) = \exp\left(-i\frac{M_a c^2}{\hbar} t\right) \cdot \psi_a(\vec{r}) , \quad (\text{II.10})$$

where the *mass eigenvalues* M_a are to be determined just by solving the mass eigenvalue problem below. Furthermore, one observes the fact that the Dirac four-spinors $\psi_a(\vec{r})$ may be conceived as the Whitney sums of Pauli two-spinors ${}^{(a)}\varphi_{\pm}(\vec{r})$, i.e. we put

$$\psi_a(\vec{r}) = {}^{(a)}\varphi_+(\vec{r}) \oplus {}^{(a)}\varphi_-(\vec{r}) ; \quad (\text{II.11})$$

and for these Pauli spinors one deduces from the original Dirac equations (II.8a)-(II.8b) the following *mass eigenvalue equations* [17]

$$i\vec{\sigma} \cdot \vec{\nabla} {}^{(1)}\varphi_{\pm}(\vec{r}) + {}^{(2)}A_0(\vec{r}) \cdot {}^{(1)}\varphi_{\mp}(\vec{r}) = \frac{\pm M + M_*}{\hbar} c \cdot {}^{(1)}\varphi_{\mp}(\vec{r}) \quad (\text{II.12a})$$

$$i\vec{\sigma} \cdot \vec{\nabla} {}^{(2)}\varphi_{\pm}(\vec{r}) + {}^{(1)}A_0(\vec{r}) \cdot {}^{(2)}\varphi_{\mp}(\vec{r}) = -\frac{M_* \pm M}{\hbar} c \cdot {}^{(2)}\varphi_{\mp}(\vec{r}) . \quad (\text{II.12b})$$

Here, the common rest mass is denoted by M , cf. (II.7), and the common mass eigenvalue by M_* ($= -M_1 = M_2$). Furthermore, we have also neglected the magnetic potentials (i.e. putting $\vec{A}_a(\vec{r}) \equiv 0 \rightsquigarrow$ *electrostatic approximation*). An essential point with this neglection of magnetism aims at the well-known ortho/para dichotomy of positronium [11]. Namely, it should be self-evident that the physical difference of ortho- and para-positronium becomes annihilated through disregarding the magnetic interaction energy, see the discussion of this in ref. [11]. But observe on the other hand that the present mass eigenvalue system (II.12a)-(II.12b) is still of truly relativistic nature, though it is written in terms of Pauli 2-spinors, not in terms of Dirac 4-spinors!

A further crucial point of the eigenvalue system (II.12a)-(II.12b) concerns the plausible assumption that, from symmetry reasons, both particles (i.e. electron and positron) will occupy the same physical quantum state (for a more detailed discussion see ref. [17]). A

nearby consequence of this assumption is that the Dirac four-densities ${}^{(a)}k_\mu(\vec{r})$ must be the same for both particles

$${}^{(1)}k_\mu(\vec{r}) = {}^{(2)}k_\mu(\vec{r}) \doteq {}^{(p)}k_\mu(\vec{r}) , \quad (\text{II.13})$$

provided the two particles do combine to the *para-state* (for the case of *ortho-positronium* see ref.s [11, 17]). On the other hand, the Dirac densities ${}^{(a)}k_0(\vec{r})$ read in terms of the Pauli spinors ${}^{(a)}\varphi_\pm(\vec{r})$ (II.11)

$${}^{(a)}k_0(\vec{r}) = {}^{(a)}\varphi_+^\dagger(\vec{r}) {}^{(a)}\varphi_+(\vec{r}) + {}^{(a)}\varphi_-^\dagger(\vec{r}) {}^{(a)}\varphi_-(\vec{r}) \quad (\text{II.14})$$

and similarly for the Dirac currents $\vec{k}_a(\vec{r})$

$$\vec{k}_a(\vec{r}) = {}^{(a)}\varphi_+^\dagger(\vec{r}) \vec{\sigma} {}^{(a)}\varphi_-(\vec{r}) + {}^{(a)}\varphi_-^\dagger(\vec{r}) \vec{\sigma} {}^{(a)}\varphi_+(\vec{r}) . \quad (\text{II.15})$$

Therefore, the physical equivalence of both one-particle states allows us to parametrize both states by only one set of Pauli spinors ${}^{(p)}\varphi_\pm(\vec{r})$ which then lets appear both original spinors ${}^{(1)}\varphi_\pm(\vec{r})$ and ${}^{(2)}\varphi_\pm(\vec{r})$ as follows:

$${}^{(p)}\varphi_+(\vec{r}) \doteq {}^{(1)}\varphi_+(\vec{r}) = i \left(\hat{\vec{k}} \cdot \vec{\sigma} \right) {}^{(2)}\varphi_+(\vec{r}) \quad (\text{II.16a})$$

$${}^{(p)}\varphi_-(\vec{r}) \doteq {}^{(1)}\varphi_-(\vec{r}) = i \left(\hat{\vec{k}} \cdot \vec{\sigma} \right) {}^{(2)}\varphi_-(\vec{r}) \quad (\text{II.16b})$$

$$\left(\hat{\vec{k}} = \frac{\vec{k}_p}{||\vec{k}_p||} \right) .$$

By use of the usual spinor algebra one can easily verify that the algebraic requirements (II.13) are actually satisfied through the present arrangements (II.16a)-(II.16b); and additionally the *two* equations (II.12a)-(II.12b) for the individual spinors ${}^{(1)}\varphi_\pm(\vec{r})$ and ${}^{(2)}\varphi_\pm(\vec{r})$ become reduced to *one* equation for the para-spinor ${}^{(p)}\varphi_\pm(\vec{r})$:

$$i\vec{\sigma} \cdot \vec{\nabla} {}^{(p)}\varphi_\pm(\vec{r}) - {}^{(p)}A_0(\vec{r}) \cdot {}^{(p)}\varphi_\mp(\vec{r}) = \frac{M_* \pm M}{\hbar} c \cdot {}^{(p)}\varphi_\mp(\vec{r}) . \quad (\text{II.17})$$

Here, both electrostatic potentials ${}^{(1)}A_0(\vec{r})$ and ${}^{(2)}A_0(\vec{r})$ have also been identified up to sign

$${}^{(1)}A_0(\vec{r}) \equiv - {}^{(2)}A_0(\vec{r}) \doteq {}^{(p)}A_0(\vec{r}) \quad (\text{II.18})$$

because they are generated by the same Dirac density ${}^{(p)}k_0(\vec{r})$

$${}^{(p)}k_0(\vec{r}) \doteq {}^{(1)}k_0(\vec{r}) \equiv {}^{(2)}k_0(\vec{r}) . \quad (\text{II.19})$$

The precise form of the link between the potential ${}^{(p)}A_0(\vec{r})$ and the Dirac density ${}^{(p)}k_0(\vec{r})$ must now be deduced from the original gauge field equations.

2. Gauge Field Subsystem

The gauge field counterpart of the basic matter field equation (II.1) is the (generally non-Abelian) Maxwell equation

$$\begin{aligned} \mathcal{D}^\mu \mathcal{F}_{\mu\nu} &= -4\pi i \alpha_s \mathcal{J}_\nu \\ \left(\alpha_s \doteq \frac{e^2}{\hbar c} \right) , \end{aligned} \quad (\text{II.20})$$

with the curvature $\mathcal{F}_{\mu\nu}$ of the bundle connection \mathcal{A}_μ (II.5) being defined as usual in the gauge field theories

$$\begin{aligned} \mathcal{F}_{\mu\nu} &\doteq \nabla_\mu \mathcal{A}_\nu - \nabla_\nu \mathcal{A}_\mu + [\mathcal{A}_\mu, \mathcal{A}_\nu] \\ &= \sum_{a=1}^2 F^a_{\mu\nu} \tau_a + G_{\mu\nu} \chi - \overset{*}{G}_{\mu\nu} \bar{\chi} . \end{aligned} \quad (\text{II.21})$$

However, for the present situation of *different* particles the exchange potential B_μ vanishes identically ($B_\mu \equiv 0$) and consequently the theory becomes Abelian with the two field strengths $F^a_{\mu\nu}$ being defined in terms of the residual electromagnetic potentials A^a_μ through ($a = 1, 2$)

$$F^a_{\mu\nu} = \nabla_\mu A^a_\nu - \nabla_\nu A^a_\mu . \quad (\text{II.22})$$

Furthermore, since we are presently satisfied with the *electrostatic approximation*, the relativistic relation (II.22) reduces to a simple gradient link of the electric field strengths $\vec{E}_a(\vec{r})$ to the electrostatic potentials ${}^{(a)}A_0(\vec{r})$

$$\vec{E}_a(\vec{r}) = -\vec{\nabla} {}^{(a)}A_0(\vec{r}) . \quad (\text{II.23})$$

From the same reason, the original Maxwell equations (II.20) do reappear as simple source relations

$$\vec{\nabla} \cdot \vec{E}_a = 4\pi\alpha_s \cdot {}^{(a)}j_0(\vec{r}) \quad (\text{II.24})$$

where however the Maxwell densities $j^a_\mu = \{ {}^{(a)}j_0, -\vec{j}_a \}$ are related to the Dirac densities $k_{a\mu}$ through

$$j^1_\mu = k_{1\mu} = \{ {}^{(1)}k_0, -\vec{k}_1 \} \quad (\text{II.25a})$$

$$j^2_\mu = -k_{2\mu} = \{ -{}^{(2)}k_0, \vec{k}_2 \} . \quad (\text{II.25b})$$

Thus the source equations (II.24) ultimately appear as the well-known Poisson equations

$$\Delta {}^{(1)}A_0 = -4\pi\alpha_s {}^{(1)}k_0 \quad (\text{II.26a})$$

$$\Delta {}^{(2)}A_0 = 4\pi\alpha_s {}^{(2)}k_0 , \quad (\text{II.26b})$$

which however are contracted to only one equation:

$$\begin{aligned} \Delta {}^{(p)}A_0(\vec{r}) &= -4\pi\alpha_s \cdot {}^{(p)}k_0(\vec{r}) \\ &= -4\pi\alpha_s \left[{}^{(p)}\varphi_+^\dagger(\vec{r}) {}^{(p)}\varphi_+(\vec{r}) + {}^{(p)}\varphi_-^\dagger(\vec{r}) {}^{(p)}\varphi_-(\vec{r}) \right] , \end{aligned} \quad (\text{II.27})$$

namely as a consequence of the former identifications (II.13) and (II.18).

Summarizing, the RST eigenvalue problem for positronium in the electrostatic approximation consists of the mass eigenvalue equation (II.17) in combination with the present Poisson equation (II.27). It is true, this is a *closed* system for the Pauli spinors ${}^{(p)}\varphi_{\pm}(\vec{r})$ and the interaction potential ${}^{(p)}A_0(\vec{r})$ but it demands the specification of certain boundary conditions. Clearly, for the matter fields one demands their sufficiently rapid vanishing at infinity ($r \rightarrow \infty$), i.e.

$$\lim_{r \rightarrow \infty} {}^{(p)}\varphi_{\pm}(\vec{r}) = 0 \Rightarrow \lim_{r \rightarrow \infty} {}^{(p)}k_0(\vec{r}) = 0 ; \quad (\text{II.28})$$

and moreover one wishes also to have thereout the asymptotic Coulomb form for the interaction potential ${}^{(p)}A_0(\vec{r})$

$$\lim_{r \rightarrow \infty} {}^{(p)}A_0(\vec{r}) = \frac{\alpha_s}{r} . \quad (\text{II.29})$$

Both conditions (II.28)-(II.29) lead us to the standard solution of the Poisson equation (II.27), i.e.

$${}^{(p)}A_0(\vec{r}) = \alpha_s \int d^3\vec{r}' \frac{{}^{(p)}k_0(\vec{r}')}{||\vec{r} - \vec{r}'||}, \quad (\text{II.30})$$

where the normalization condition for the Pauli spinors

$$\int d^3\vec{r} {}^{(p)}k_0(\vec{r}) = 1 \quad (\text{II.31})$$

(cf. (II.14)) actually ensures the asymptotic Coulomb form (II.29) of the potential ${}^{(p)}A_0(\vec{r})$ (II.30).

3. Energy Functional

Even if one would be able to find exact solutions of the eigenvalue equations (II.17) plus (II.27), with both constraints (II.29) and (II.31) being obeyed, one nevertheless would be forced to face the problem of the energy content carried by that elaborated solutions. In other words, one needs an energy functional ($\tilde{E}_{[T]}$, say) whose value upon the constructed solution yields its physically relevant and observable energy. Surely, the wanted energy E_T cannot be identified with the mass eigenvalue M_*c^2 because this quantity refers separately to each of both particles and therefore is a one-particle quantity whereas we would like to know the total energy E_T of the *interactive* two-particle system. It would also not help to take $2M_*c^2$ as the desired energy E_T because M_*c^2 alone does already contain the whole electrostatic interaction energy which then would be counted twice.

The solution of this energy problem has been already worked out in some precedent papers [11] and for the sake of brevity it may suffice here to simply quote the result:

$$\tilde{E}_{[T]} = E_{[T]}^{(\text{IV})} + 2\lambda_D \cdot N_D + \lambda_G^{(e)} \cdot N_G^{(e)}. \quad (\text{II.32})$$

This general form of the energy functional says that there are essentially two parts which are equipped with a rather different meaning: the first part $E_{[T]}^{(\text{IV})}$ is a collection of the

truly physical energy contributions

$$E_{[T]}^{(IV)} = 2Mc^2 \cdot \mathcal{Z}_\varphi^2 + 4^{(p)}T_{\text{kin}} + E_R^{(e)} \quad (\text{II.33})$$

while the second part does refer to the constraints.

Here the first constraint (N_D) refers to the wave function normalization (II.31):

$$N_D \doteq \int d^3\vec{r} \left({}^{(p)}\varphi_+^\dagger {}^{(p)}\varphi_+ + {}^{(p)}\varphi_-^\dagger {}^{(p)}\varphi_- \right) - 1 \equiv 0 , \quad (\text{II.34})$$

and λ_D is the associated Lagrangean multiplier. Similarly, the second constraint ($N_G^{(e)}$) does refer to the *Poisson identity*

$$N_G^{(e)} \doteq E_R^{(e)} - M^{(e)}c^2 \equiv 0 \quad (\text{II.35})$$

with the gauge field energy $E_R^{(e)}$ being defined through

$$E_R^{(e)} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3\vec{r} \left(\vec{E}_p \cdot \vec{E}_p \right) \quad (\text{II.36})$$

and its mass equivalent ($M^{(e)}c^2$) through

$$M^{(e)}c^2 = -\hbar c \int d^3\vec{r} {}^{(p)}A_0(\vec{r}) \cdot {}^{(p)}k_0(\vec{r}) . \quad (\text{II.37})$$

The Poisson identity (II.35) itself is an immediate consequence of the Poisson equation (II.27) and therefore is automatically satisfied not only for the exact solutions of the RST eigenvalue problem but also for its approximate solutions (see below) if only the approximate potential ${}^{(p)}A_0(\vec{r})$ is linked to the (approximate) Dirac density ${}^{(p)}k_0(\vec{r})$ via the Poisson equation (II.27). Thus, if one takes care of satisfying simultaneously both constraints (II.34) and (II.35) the energy functional $\tilde{E}_{[T]}$ (II.32) becomes reduced to its physical part $E_{[T]}^{(IV)}$ (II.33).

This latter part (II.33) represents the proper physical content of the energy functional $\tilde{E}_{[T]}$ and consists of the (renormalized) rest mass energy, the kinetic energy of both particles and the gauge field energy $E_R^{(e)}$ (II.36). The mass renormalization factor \mathcal{Z}_φ is given by

$$\mathcal{Z}_\varphi^2 = \int d^3\vec{r} \left({}^{(p)}\varphi_+^\dagger {}^{(p)}\varphi_+ - {}^{(p)}\varphi_-^\dagger {}^{(p)}\varphi_- \right) , \quad (\text{II.38})$$

and the one-particle kinetic energy ${}^{(p)}T_{\text{kin}}$ reads

$${}^{(p)}T_{\text{kin}} = i \frac{\hbar c}{2} \int d^3 \vec{r} \left[{}^{(p)}\varphi_+^\dagger(\vec{r}) (\vec{\sigma} \cdot \vec{\nabla}) {}^{(p)}\varphi_-(\vec{r}) + {}^{(p)}\varphi_-^\dagger(\vec{r}) (\vec{\sigma} \cdot \vec{\nabla}) {}^{(p)}\varphi_+(\vec{r}) \right]. \quad (\text{II.39})$$

After all, it is a nice consistency check to carry explicitly through that standard recipe of variational calculus as it is required by the *principle of minimal energy*

$$\delta \tilde{E}_{[\text{T}]} = 0. \quad (\text{II.40})$$

Or in other words, the extremalization of the energy functional $\tilde{E}_{[\text{T}]}$ (II.32) with respect to the Pauli spinors ${}^{(p)}\varphi_\pm^\dagger, {}^{(p)}\varphi_\pm$ yields just the mass eigenvalue equations (II.17) as the first part of the RST eigenvalue problem; and analogously the extremalization of $\tilde{E}_{[\text{T}]}$ (II.32) with respect to the electrostatic potential ${}^{(p)}A_0(\vec{r})$ lets one recover the Poisson equation (II.27), provided both constraints (II.34) and (II.35) are duly regarded.

III Spherically Symmetric Approximation

From the preceding presentation of the RST eigenvalue problem it should be evident that it is (almost) impossible to construct exact solutions of such a peculiar kind of eigenvalue problem. On the other hand, it is perhaps not even necessary to know those exact solutions since their main features could possibly be grasped already by studying certain *approximate* solutions. A nearby simplification as the basis for such an approximative approach refers to those anisotropic effects which are invading the calculations via the spin degree of freedom inherent in the Dirac equations. In order to get rid of this type of complication, one may neglect the anisotropic influence of the spin on the electrostatic interaction potential and may assume that the interaction potential ${}^{(p)}A_0(\vec{r})$ is nearly spherically symmetric, i.e. we put

$$\begin{aligned} {}^{(p)}A_0(\vec{r}) &\Rightarrow [{}^p]A_0(r) \\ &\left(r = \|\vec{r}\| \right), \end{aligned} \tag{III.1}$$

where this assumption of spherical symmetry needs not be applied to the wave amplitudes of the particles themselves. For such a first estimate of the positronium spectrum (on the level of accuracy of the conventional treatment (I.4)) it is also not necessary to stick to the relativistic formulation of the theory, but rather one may again be satisfied with the non-relativistic limit. Thus we will first eliminate the explicit spin anisotropy effect from the eigenvalue problem and afterwards we will resort to the non-relativistic approximation.

1. Double-Valued Spinor Fields

The manifest spin degree of freedom may be eliminated by first parametrizing the Pauli spinors ${}^{(p)}\varphi_{\pm}(\vec{r})$ through the *wave amplitudes* ${}^{(p)}\mathcal{R}_{\pm}(\vec{r})$ and ${}^{(p)}\mathcal{S}_{\pm}(\vec{r})$ as the components of ${}^{(p)}\varphi_{\pm}(\vec{r})$ with respect to a selected spinor basis; next, one separates off their angular parts and finally one impresses a *rigid* link on the remaining radial parts of both

amplitudes ${}^{(p)}\mathcal{R}_\pm(\vec{r})$ and ${}^{(p)}\mathcal{S}_\pm(\vec{r})$. This procedure yields (in its non-relativistic version) a scalar eigenvalue problem of the Schrödinger type, see equation (III.34) below.

The selection of an appropriate spinor basis starts with the standard eigenspinors $\zeta_l^{j,m}$ of total angular momentum $\hat{\vec{J}} (= \hat{\vec{L}} + \hat{\vec{S}})$ in two-dimensional unitary space

$$\hat{\vec{J}}^2 \zeta_l^{j,m} = j(j+1)\hbar^2 \cdot \zeta_l^{j,m} \quad (\text{III.2a})$$

$$\hat{\vec{L}}^2 \zeta_l^{j,m} = l(l+1)\hbar^2 \cdot \zeta_l^{j,m} \quad (\text{III.2b})$$

$$\hat{\vec{S}}^2 \zeta_l^{j,m} = s(s+1)\hbar^2 \cdot \zeta_l^{j,m} = \frac{1}{2} \left(\frac{1}{2} + 1 \right) \hbar^2 \cdot \zeta_l^{j,m} \quad (\text{III.2c})$$

$$\hat{J}_z \zeta_l^{j,m} = m\hbar \cdot \zeta_l^{j,m} . \quad (\text{III.2d})$$

For the sake of simplicity, one may prefer here $l = 0, 1$ for the orbital part of angular momentum so that $\{\zeta_0^{\frac{1}{2}, \pm\frac{1}{2}}\}$ could be a basis for the “positive” Pauli spinors ${}^{(p)}\varphi_+(\vec{r})$ and similarly $\{\zeta_1^{\frac{1}{2}, \pm\frac{1}{2}}\}$ a basis for the “negative” spinors ${}^{(p)}\varphi_-(\vec{r})$. Now one can show that (for para-positronium (II.16a)-(II.16b)) the action of the z-component \hat{J}_z of total angular momentum $\hat{\vec{J}}$ must annihilate both spinors ${}^{(p)}\varphi_\pm(\vec{r})$, i.e.

$$\hat{J}_z^{(+)} {}^{(p)}\varphi_+(\vec{r}) = 0 \quad (\text{III.3a})$$

$$\hat{J}_z^{(-)} {}^{(p)}\varphi_-(\vec{r}) = 0 , \quad (\text{III.3b})$$

see ref.s [11, 17]. Or in other words, the action of the total operator $\hat{\mathcal{J}}_z$ ($\doteqdot \hat{J}_z^{(+)} \oplus \hat{J}_z^{(-)}$) annihilates the one-particle Dirac spinor field ψ_φ ($\doteqdot {}^{(p)}\varphi_+ \oplus {}^{(p)}\varphi_-$), i. e.

$$\hat{\mathcal{J}}_z \psi_\varphi = 0 . \quad (\text{III.4})$$

But clearly, such a one-particle state must be of rather exotic nature because an ordinary (“fermionic”) Dirac eigenspinor of $\hat{\mathcal{J}}_z$ has always half-integer eigenvalue; and consequently such a strange (“bosonic”) state as (III.4) must own some unusual property. Indeed this concerns its uniqueness in the sense that the spinor field ψ_φ (III.3a)-(III.4) is *double-valued* [11, 17]

$$\psi_\varphi(r, \vartheta, \phi + 2\pi) = -\psi_\varphi(r, \vartheta, \phi) \quad (\text{III.5})$$

where r, ϑ, ϕ are the usual spherical polar coordinates of flat three-space. On the other hand, both basis systems $\{\zeta_0^{\frac{1}{2}, \pm\frac{1}{2}}\}$ and $\{\zeta_1^{\frac{1}{2}, \pm\frac{1}{2}}\}$ (III.2a)-(III.2d) are unique over three-space; and thus if one would decompose such a spinor-like ψ_φ (III.5) with respect to a standard basis, the corresponding components would have to be non-unique scalar fields over three-space. However, our option is here just the other way round, namely to choose certain basis systems $\omega_0^{(\pm)}$ and $\omega_1^{(\pm)}$ which themselves carry the double-valuedness (III.5) *alone* so that the components of ψ_φ can remain unique scalar fields, i.e.

$$\omega_0^{(\pm)}(r, \vartheta, \phi + 2\pi) = -\omega_0^{(\pm)}(r, \vartheta, \phi) \quad (\text{III.6a})$$

$$\omega_1^{(\pm)}(r, \vartheta, \phi + 2\pi) = -\omega_1^{(\pm)}(r, \vartheta, \phi) . \quad (\text{III.6b})$$

Now our choice of basis system looks as follows:

$$\omega_0^{(+)} = e^{-i\frac{\phi}{2}} \cdot \zeta_0^{\frac{1}{2}, \frac{1}{2}} \quad (\text{III.7a})$$

$$\omega_0^{(-)} = e^{i\frac{\phi}{2}} \cdot \zeta_0^{\frac{1}{2}, -\frac{1}{2}} \quad (\text{III.7b})$$

$$\omega_1^{(+)} = e^{-i\frac{\phi}{2}} \cdot \zeta_1^{\frac{1}{2}, \frac{1}{2}} \quad (\text{III.7c})$$

$$\omega_1^{(-)} = e^{i\frac{\phi}{2}} \cdot \zeta_1^{\frac{1}{2}, -\frac{1}{2}} , \quad (\text{III.7d})$$

so that this ω -basis becomes annihilated by $\hat{J}_z^{(\pm)}$:

$$\hat{J}_z^{(+)} \omega_0^{(\pm)} = 0 \quad (\text{III.8a})$$

$$\hat{J}_z^{(-)} \omega_1^{(\pm)} = 0 . \quad (\text{III.8b})$$

The double-valuedness (III.6a)-(III.6b) of the chosen basis system transcribes now to the Pauli spinors ${}^{(p)}\varphi_{\pm}(\vec{r})$, provided one adopts the corresponding components ${}^{(p)}\mathcal{R}_{\pm}$, ${}^{(p)}\mathcal{S}_{\pm}$ to be unique. Accordingly, the desired decomposition reads

$${}^{(p)}\varphi_+(\vec{r}) = {}^{(p)}\mathcal{R}_+(\vec{r}) \cdot \omega_0^{(+)} + {}^{(p)}\mathcal{S}_+(\vec{r}) \cdot \omega_0^{(-)} \quad (\text{III.9a})$$

$${}^{(p)}\varphi_-(\vec{r}) = -i \left\{ {}^{(p)}\mathcal{R}_-(\vec{r}) \cdot \omega_1^{(+)} + {}^{(p)}\mathcal{S}_-(\vec{r}) \cdot \omega_1^{(-)} \right\} \quad (\text{III.9b})$$

with *unique* scalar components

$${}^{(p)}\mathcal{R}_{\pm}(r, \vartheta, \phi + 2\pi) = {}^{(p)}\mathcal{R}_{\pm}(r, \vartheta, \phi) \quad (\text{III.10a})$$

$${}^{(p)}\mathcal{S}_{\pm}(r, \vartheta, \phi + 2\pi) = {}^{(p)}\mathcal{S}_{\pm}(r, \vartheta, \phi) . \quad (\text{III.10b})$$

2. Eigenvalue Equations for the Wave Amplitudes

Further information about the components ${}^{(p)}\mathcal{R}_{\pm}(\vec{r})$ and ${}^{(p)}\mathcal{S}_{\pm}(\vec{r})$ can be gained by inspection of how the annihilation process (III.3a)-(III.3b) can be realized in detail. Indeed, a straightforward calculation yields

$$\hat{J}_z^{(+)} {}^{(p)}\varphi_+(\vec{r}) = (\hat{L}_z {}^{(p)}\mathcal{R}_+) \cdot \omega_0^{(+)} + (\hat{L}_z {}^{(p)}\mathcal{S}_+) \cdot \omega_0^{(-)} + {}^{(p)}\mathcal{R}_+ \cdot (\hat{J}_z^{(+)} \omega_0^{(+)}) + {}^{(p)}\mathcal{S}_+ \cdot (\hat{J}_z^{(+)} \omega_0^{(-)}) \quad (\text{III.11})$$

and analogously for ${}^{(p)}\varphi_-(\vec{r})$. Observing here the annihilation relations for the ω -basis (III.8a)-(III.8b) it is clear that one has to demand

$$\hat{L}_z {}^{(p)}\mathcal{R}_+ = \hat{L}_z {}^{(p)}\mathcal{S}_+ = 0 \quad (\text{III.12})$$

in order to have the eigenvalue equations (III.3a)-(III.3b) for angular momentum satisfied. However, the latter demand (III.12) can trivially be satisfied by letting the wave amplitudes ${}^{(p)}\mathcal{R}_{\pm}(\vec{r})$, ${}^{(p)}\mathcal{S}_{\pm}(\vec{r})$ depend exclusively upon r and ϑ , but not on ϕ . Thus one puts

$${}^{(p)}\mathcal{R}_{\pm}(\vec{r}) \Rightarrow {}^{(p)}R_{\pm}(r, \vartheta) \quad (\text{III.13a})$$

$${}^{(p)}\mathcal{S}_{\pm}(\vec{r}) \Rightarrow {}^{(p)}S_{\pm}(r, \vartheta) . \quad (\text{III.13b})$$

Furthermore, it turns out that the equations for the wave amplitudes become considerably simplified if one resorts to a further transformation:

$${}^{(p)}R_{\pm}(r, \vartheta) = \frac{{}^{(p)}\tilde{R}_{\pm}(r, \vartheta)}{\sqrt{r \sin \vartheta}} \quad (\text{III.14a})$$

$${}^{(p)}S_{\pm}(r, \vartheta) = \frac{{}^{(p)}\tilde{S}_{\pm}(r, \vartheta)}{\sqrt{r \sin \vartheta}} . \quad (\text{III.14b})$$

Namely, the relativistic Pauli equations (II.12a)-(II.12b) are then recast to the following relatively simple eigenvalue equations for the new amplitudes ${}^{(p)}\tilde{R}_\pm$, ${}^{(p)}\tilde{S}_\pm$ [11]

$$\frac{\partial {}^{(p)}\tilde{R}_+}{\partial r} + \frac{1}{r} \frac{\partial {}^{(p)}\tilde{S}_+}{\partial \vartheta} - {}^{(p)}A_0 \cdot {}^{(p)}\tilde{R}_- = \frac{M + M_*}{\hbar} c \cdot {}^{(p)}\tilde{R}_- \quad (\text{III.15a})$$

$$\frac{\partial {}^{(p)}\tilde{S}_+}{\partial r} - \frac{1}{r} \frac{\partial {}^{(p)}\tilde{R}_+}{\partial \vartheta} - {}^{(p)}A_0 \cdot {}^{(p)}\tilde{S}_- = \frac{M + M_*}{\hbar} c \cdot {}^{(p)}\tilde{S}_- \quad (\text{III.15b})$$

$$\frac{\partial {}^{(p)}\tilde{R}_-}{\partial r} + \frac{1}{r} \cdot {}^{(p)}\tilde{R}_- - \frac{1}{r} \frac{\partial {}^{(p)}\tilde{S}_-}{\partial \vartheta} + {}^{(p)}A_0 \cdot {}^{(p)}\tilde{R}_+ = \frac{M - M_*}{\hbar} c \cdot {}^{(p)}\tilde{R}_+ \quad (\text{III.15c})$$

$$\frac{\partial {}^{(p)}\tilde{S}_-}{\partial r} + \frac{1}{r} \cdot {}^{(p)}\tilde{S}_- + \frac{1}{r} \frac{\partial {}^{(p)}\tilde{R}_-}{\partial \vartheta} + {}^{(p)}A_0 \cdot {}^{(p)}\tilde{S}_+ = \frac{M - M_*}{\hbar} c \cdot {}^{(p)}\tilde{S}_+ . \quad (\text{III.15d})$$

In order to deal with a closed system of equations for the new amplitudes, one substitutes the Pauli spinors (III.9a)-(III.9b) into the Poisson equation (II.27) which lets reappear this equation now in the following form

$$\Delta {}^{(p)}A_0 = -\alpha_s \frac{{}^{(p)}\tilde{R}_+^2 + {}^{(p)}\tilde{S}_+^2 + {}^{(p)}\tilde{R}_-^2 + {}^{(p)}\tilde{S}_-^2}{r \sin \vartheta}. \quad (\text{III.16})$$

The coupled system (III.15a)-(III.16) represents now the RST eigenvalue problem for para-positronium in the electrostatic approximation; but despite its simplified form it is hard (or even impossible) to elaborate the exact solutions hereof.

3. Spherical Symmetry

In this situation, the approximative assumption of spherical symmetry (III.1) allows further progress. Namely, it is just this assumption which suggests to try a product ansatz for the wave amplitudes of the following form [11]

$${}^{(p)}\tilde{R}_\pm(r, \vartheta) = 'R_\pm(r) \cdot f_R(\vartheta) \quad (\text{III.17a})$$

$${}^{(p)}\tilde{S}_\pm(r, \vartheta) = 'S_\pm(r) \cdot f_S(\vartheta) . \quad (\text{III.17b})$$

Indeed, substituting this ansatz into the mass eigenvalue equations (III.15a-III.15d) allows one to separate the variables so that there emerges one subset of equations for the radial functions $'R_{\pm}(r)$, $'S_{\pm}(r)$ and one subset for the angular functions $f_R(\vartheta)$ and $f_S(\vartheta)$. Here, the angular equations introduce the quantum number l_{\wp} of orbital angular momentum in the following way:

$$\frac{df_R(\vartheta)}{d\vartheta} = l_{\wp} \cdot f_S(\vartheta) \quad (\text{III.18a})$$

$$\frac{df_S(\vartheta)}{d\vartheta} = -l_{\wp} \cdot f_R(\vartheta), \quad (\text{III.18b})$$

where a second possibility does exist which, however, has merely the sign of l_{\wp} reversed (i. e. $l_{\wp} \Rightarrow -l_{\wp}$). The separated angular problem (III.18a)-(III.18b) is so simple that its solutions are immediately evident, namely either

$$f_R(\vartheta) = \cos(l_{\wp} \cdot \vartheta), \quad f_S(\vartheta) = -\sin(l_{\wp} \cdot \vartheta) \quad (\text{III.19})$$

or

$$f_R(\vartheta) = \sin(l_{\wp} \cdot \vartheta), \quad f_S(\vartheta) = \cos(l_{\wp} \cdot \vartheta), \quad (\text{III.20})$$

with the quantum number l_{\wp} adopting (half-)integer values

$$l_{\wp} = 0, \left(\frac{1}{2}\right), 1, \left(\frac{3}{2}\right), 2, \left(\frac{5}{2}\right), 3, \dots \quad (\text{III.21})$$

This postulate of (half-)integrity follows from the demand that the Dirac current \vec{k}_p remains finite on the z -axis ($\vartheta = 0, \pi$). For the exclusion of the half-integers see below.

After the angular part is split off in that way (III.17a)-(III.17b), there remains a purely radial problem for the determination of the mass eigenvalue M_* . Indeed, substituting the separation ansatz (III.17a)-(III.17b) back into the original eigenvalue equations (III.15a)-(III.15d) and using also the angular equations (III.18a)-(III.18b) yields the following set

of coupled radial equations:

$$\frac{d'R_+(r)}{dr} - \frac{l_\varphi}{r} \cdot 'S_+(r) - {}^{[p]}A_0(r) \cdot 'R_-(r) = \frac{M + M_*}{\hbar} c \cdot 'R_-(r) \quad (\text{III.22a})$$

$$\frac{d'S_+(r)}{dr} - \frac{l_\varphi}{r} \cdot 'R_+(r) - {}^{[p]}A_0(r) \cdot 'S_-(r) = \frac{M + M_*}{\hbar} c \cdot 'S_-(r) \quad (\text{III.22b})$$

$$\frac{d'R_-(r)}{dr} + \frac{1}{r} \cdot 'R_-(r) + \frac{l_\varphi}{r} \cdot 'S_-(r) + {}^{[p]}A_0(r) \cdot 'R_+(r) = \frac{M - M_*}{\hbar} c \cdot 'R_+(r) \quad (\text{III.22c})$$

$$\frac{d'S_-(r)}{dr} + \frac{1}{r} \cdot 'S_-(r) + \frac{l_\varphi}{r} \cdot 'R_-(r) + {}^{[p]}A_0(r) \cdot 'S_+(r) = \frac{M - M_*}{\hbar} c \cdot 'S_+(r) . \quad (\text{III.22d})$$

Surely, it appears somewhat strange here that one and the same eigenvalue M_* enters all four equations (III.22a)-(III.22d); but this may be understood as a hint at the circumstance that there exists a rigid link between the four variables $'R_{\pm}(r)$, $'S_{\pm}(r)$. And indeed, the following identifications

$$'R_+(r) \equiv 'S_+(r) \doteqdot \tilde{\Phi}_+(r) \quad (\text{III.23a})$$

$$'R_-(r) \equiv 'S_-(r) \doteqdot \tilde{\Phi}_-(r) \quad (\text{III.23b})$$

recast this system of four equations to only two equations

$$\frac{d\tilde{\Phi}_+(r)}{dr} - \frac{l_\varphi}{r} \cdot \tilde{\Phi}_+(r) - {}^{[p]}A_0(r) \cdot \tilde{\Phi}_-(r) = \frac{M + M_*}{\hbar} c \cdot \tilde{\Phi}_-(r) \quad (\text{III.24a})$$

$$\frac{d\tilde{\Phi}_-(r)}{dr} + \frac{l_\varphi + 1}{r} \cdot \tilde{\Phi}_-(r) + {}^{[p]}A_0(r) \cdot \tilde{\Phi}_+(r) = \frac{M - M_*}{\hbar} c \cdot \tilde{\Phi}_+(r) . \quad (\text{III.24b})$$

This spherically symmetric eigenvalue problem may finally be completed by the corresponding Poisson equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) {}^{[p]}A_0(r) = -\frac{\pi}{2} \alpha_s \frac{\tilde{\Phi}_+^2(r) + \tilde{\Phi}_-^2(r)}{r} \quad (\text{III.25})$$

which is to be conceived as the spherically symmetric simplification of (III.16). Notice here also the important fact that the quantum number l_φ does not explicitly enter the source terms of the spherically symmetric Poisson equation (III.25)! The standard solution of this type of equation reads formally

$${}^{[p]}A_0(r) = \frac{\alpha_s}{8} \int \frac{d^3\vec{r}'}{r'} \frac{\tilde{\Phi}_+^2(r') + \tilde{\Phi}_-^2(r')}{\|\vec{r} - \vec{r}'\|} \quad (\text{III.26})$$

and approaches the Coulomb potential at infinity ($r \rightarrow \infty$), i.e.

$$\lim_{r \rightarrow \infty} {}^{[p]}A_0(r) = \frac{\alpha_s}{r} , \quad (\text{III.27})$$

namely just on account of the normalization condition (II.31) which reads in terms of the wave amplitudes $\tilde{\Phi}_{\pm}(r)$

$$\frac{\pi}{2} \int dr' r' \left\{ \tilde{\Phi}_+^2(r') + \tilde{\Phi}_-^2(r') \right\} = 1 . \quad (\text{III.28})$$

Clearly, such a requirement can only be satisfied if the amplitudes $\tilde{\Phi}_{\pm}(r)$ obey the usual boundary condition

$$\lim_{r \rightarrow \infty} \tilde{\Phi}_{\pm}(r) = 0 . \quad (\text{III.29})$$

However, a somewhat more critical point concerning the boundary conditions refers to the behaviour of the angular functions $f_R(\vartheta)$ and $f_S(\vartheta)$ (III.19)-(III.20) on the z -axis (i.e. $\vartheta = 0, \pi$). From generally accepted arguments one would think that all physically relevant objects of the theory should be non-singular everywhere. In the present context, the crucial object is here the Dirac current \vec{k}_p which for the presently considered kinematics of the Dirac spinor field $\psi_{\phi} = {}^{(p)}\varphi_+ \oplus {}^{(p)}\varphi_-$ encircles the z -axis

$$\vec{k}_p(\vec{r}) = {}^{(p)}k_{\phi}(r, \vartheta) \cdot \vec{e}_{\phi} \quad (\text{III.30})$$

with the azimuthal component being given by

$${}^{(p)}k_{\phi}(r, \vartheta) = \pm \frac{\tilde{\Phi}_+(r) \cdot \tilde{\Phi}_-(r)}{2\pi r} \cdot \frac{\sin[(2l_{\phi} + 1) \cdot \vartheta]}{\sin \vartheta} . \quad (\text{III.31})$$

Therefore, if one wishes to keep this current component finite on the z -axis then one is forced to demand that l_{ϕ} can adopt only (half-)integer values, cf. (III.21). Furthermore, if one demands that ${}^{(p)}k_{\phi}$ should be distributed symmetrically along the z -axis, i.e.

$${}^{(p)}k_{\phi}(r, 0) \stackrel{!}{=} {}^{(p)}k_{\phi}(r, \pi) \quad \forall r , \quad (\text{III.32})$$

then one can admit only integer values of l_{ϕ}

$$l_{\phi} = 0, 1, 2, 3, \dots \quad (\text{III.33})$$

(For a sketch of ${}^{(p)}k_\phi$ for integer and half-integer l_ϕ , see fig. 1 of ref. [11]). Henceforth we will prefer the present quantization prescription (III.33) over the former one [11]).

But with the eigenvalue and Poisson equations (III.24a)-(III.25) being fixed now together with all the boundary conditions, one could in principle look for the solutions of this eigenvalue problem and determine the corresponding binding energies. However, it seems meaningful to first resort to a further (but ultimate) approximation.

4. Non-Relativistic Approximation

Besides the electrostatic and spherically symmetric approximations one can now take into account a final simplification, i.e. the non-relativistic limit. The point with this approximation is namely that the relativistic corrections may well be of the same order of magnitude as the magnetic effects; and therefore it seems somewhat inconsequential to neglect the magnetic effects on the one hand but on the other hand to cling to a fully relativistic formulation. Thus one should be willing now to pass over to the non-relativistic approximation of the relativistic eigenvalue system (III.24a)-(III.25). Here, the two mass eigenvalue equations (III.24a)-(III.24b) contract to only one equation for the “positive” Pauli spinor $\tilde{\Phi}_+(r)$ which for the sake of brevity is simply termed as $\tilde{\Phi}(r)$ and has then to obey the following Schrödinger-like equation:

$$-\frac{\hbar^2}{2M} \left\{ \frac{d^2\tilde{\Phi}(r)}{dr^2} + \frac{1}{r} \frac{d\tilde{\Phi}(r)}{dr} \right\} + \frac{\hbar^2}{2M} \frac{l_\phi^2}{r^2} \tilde{\Phi}(r) - \hbar c {}^{(p)}A_0(r) \cdot \tilde{\Phi}(r) = E_* \cdot \tilde{\Phi}(r) . \quad (\text{III.34})$$

The Schrödinger eigenvalue E_* emerging here is related to the former relativistic mass eigenvalue M_* by

$$E_* = (M_* - M)c^2 , \quad (\text{III.35})$$

and the meaning of l_ϕ as a quantum number of orbital angular momentum becomes now evident. In order to have the non-relativistic eigenvalue system closed, the Schrödinger

equation (III.34) must be accompanied by the non-relativistic version of the Poisson equation (III.25), i. e.

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right\} [p]A_0(r) = -\frac{\pi}{2} \alpha_s \frac{\tilde{\Phi}^2(r)}{r} . \quad (\text{III.36})$$

Correspondingly, the non-relativistic approximation of the former solution (III.26) for $[p]A_0(r)$ appears now as

$$[p]A_0(r) = \frac{\alpha_s}{8} \int \frac{d^3\vec{r}'}{r'} \frac{\tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|} \quad (\text{III.37})$$

and thus continues to obey the same Coulomb-like boundary condition (III.27), namely on account of the non-relativistic form of the normalization condition (III.28)

$$\frac{\pi}{2} \int dr r \tilde{\Phi}^2(r) = 1 . \quad (\text{III.38})$$

In this way, one finally has arrived at a well-defined non-relativistic eigenvalue problem.

But even if one were able to solve exactly this radically simplified problem, one would still be left with the problem of the energy (E_T , say) being concentrated in this field configuration. This is the question of the right energy functional $\tilde{E}_{[T]}$ whose value upon the solutions of the eigenvalue problem is required to not only yield the desired energy E_T but whose extremal equations are also required to just coincide with the eigenvalue equations:

$$\delta \tilde{E}_{[T]} = 0 . \quad (\text{III.39})$$

This *principle of minimal energy* can then also be used in order to construct *approximate* variational solutions of the eigenvalue problem; namely by guessing some trial configuration with a certain number of variational parameters $\{\beta; \nu_1, \nu_2, \dots, \nu_k\}$. The value of the non-relativistic version $\tilde{E}_{[T]}$ of the relativistic energy functional $\tilde{E}_{[T]}$ upon this trial configuration yields then an *energy function* $\mathbb{E}^{(IV)}(\beta; \nu_1, \nu_2, \dots, \nu_k)$ whose (local) extremal

values are determined by the vanishing of all the first-order derivatives

$$\begin{aligned} \frac{\partial \mathbb{E}^{(IV)}(\beta; \nu_1, \nu_2, \dots \nu_k)}{\partial \beta} &= 0 \\ \frac{\partial \mathbb{E}^{(IV)}(\beta; \nu_1, \nu_2, \dots \nu_k)}{\partial \nu_1} &= 0 \\ &\vdots \\ \frac{\partial \mathbb{E}^{(IV)}(\beta; \nu_1, \nu_2, \dots \nu_k)}{\partial \nu_k} &= 0 . \end{aligned} \quad (\text{III.40})$$

The corresponding extremal values $\mathbb{E}_*^{(IV)}$ do then specify the energy levels of the bound system, albeit only in the *non-relativistic, electrostatic and spherically symmetric* approximation!

The desired energy functional $\tilde{\mathbb{E}}_{[T]}$ is the non-relativistic version of the former $\tilde{E}_{[T]}$ (II.32)-(II.33) and has already been deduced in full detail in the preceding paper (see equation (VI.50) of ref. [11])

$$\tilde{\mathbb{E}}_{[T]} \Rightarrow \tilde{\mathbb{E}}_{[\Phi]} = 2E_{\text{kin}} + E_R^{[e]} + 2\lambda_S \tilde{N}_\Phi + \lambda_G^{(e)} \tilde{N}_G^{(e)} . \quad (\text{III.41})$$

Here, the first term represents the kinetic energy for the two particles where the one-particle energy E_{kin} is the sum of the radial part ${}^{(r)}E_{\text{kin}}$ and the longitudinal part ${}^{(\vartheta)}E_{\text{kin}}$, i. e.

$$E_{\text{kin}} = {}^{(r)}E_{\text{kin}} + {}^{(\vartheta)}E_{\text{kin}} , \quad (\text{III.42})$$

with the radial part being given by

$${}^{(r)}E_{\text{kin}} = \frac{\hbar^2}{2M} \cdot \frac{\pi}{2} \int_0^\infty dr r \left(\frac{d\tilde{\Phi}(r)}{dr} \right)^2 \quad (\text{III.43})$$

and similarly the longitudinal part by

$${}^{(\vartheta)}E_{\text{kin}} = \frac{\hbar^2}{2M} l_\varphi^2 \cdot \frac{\pi}{2} \int_0^\infty \frac{dr}{r} \tilde{\Phi}^2(r) . \quad (\text{III.44})$$

Next, the energy content $E_R^{[e]}$ of the spherically symmetric potential ${}^{[p]}A_0(r)$ reads

$$E_R^{[e]} = -\frac{\hbar c}{\alpha_s} \int_0^\infty dr \left(r \cdot \frac{d {}^{[p]}A_0(r)}{dr} \right)^2 \quad (\text{III.45})$$

and thus the physical part of the functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) consists just of these three energy contributions (III.43)-(III.45).

The residual two terms in (III.41) are constraints with Lagrangean parameters λ_S and $\lambda_G^{(e)}$. The first constraint refers to the normalization (III.38) of the non-relativistic wave amplitude $\tilde{\Phi}(r)$

$$\tilde{N}_\Phi \doteq \frac{\pi}{2} \int_0^\infty dr r \tilde{\Phi}^2(r) - 1 \equiv 0 , \quad (\text{III.46})$$

and the second constraint is the *Poisson identity*

$$\tilde{N}_G^{[e]} \doteq E_R^{[e]} - \tilde{M}^{[e]} c^2 = 0 \quad (\text{III.47})$$

with the mass equivalent $\tilde{M}^{[e]} c^2$ due to the gauge field energy $E_R^{[e]}$ being given by

$$\tilde{M}^{[e]} c^2 \doteq -\frac{\pi}{2} \hbar c \int_0^\infty dr r {}^{[p]}A_0(r) \cdot \tilde{\Phi}^2(r) . \quad (\text{III.48})$$

A nice check of all these assertions consists now in deducing the present eigenvalue system (III.34) plus (III.36) from the non-relativistic version ($\delta \tilde{\mathbb{E}}_{[\Phi]} = 0$) of the *principle of minimal energy* (III.39) by means of the standard variational techniques. Thereby the Lagrangean parameters turn out as

$$\lambda_S = -E_* \quad (\text{III.49a})$$

$$\lambda_G^{(e)} = -2 . \quad (\text{III.49b})$$

This calculus of variations may now be exploited in order to compute approximately the non-relativistic energy spectrum of positronium.

5. Spherically Symmetric Spectrum

In order to present such an example for the energy spectrum due to the spherically symmetric approximation, one may select as trial amplitude $\tilde{\Phi}(r)$ the following function:

$$\tilde{\Phi}(r) = \Phi_* r^\nu e^{-\beta r}, \quad (\text{III.50})$$

where the normalization condition (III.46) fixes the constant Φ_* to

$$\Phi_*^2 = \frac{2}{\pi} \cdot \frac{(2\beta)^{2\nu+2}}{\Gamma(2\nu+2)}. \quad (\text{III.51})$$

This trial amplitude (III.50) has only two variational parameters (i.e. β and ν), and therefore one cannot expect that the corresponding approximate energy spectrum will turn out to be more accurate than up to some few percent ($\lesssim 10\%$, say). Nevertheless this order of accuracy should be sufficient in order to estimate the magnitude of the anisotropic corrections which, plausibly, will be found to be somewhat smaller than the error induced by just the spherically symmetric approximation. In any case, once the trial amplitude $\tilde{\Phi}(r)$ is fixed, one can proceed to determine the value of the non-relativistic energy functional $\tilde{\mathbb{E}}_{[T]}$ upon this trial configuration which then yields the corresponding energy function $\mathbb{E}^{(\text{IV})}(\beta, \nu)$ through the following steps:

- (i) Calculate the kinetic energy E_{kin} (III.42)-(III.44) by means of the selected trial function $\tilde{\Phi}(r)$ (III.50) and find this quantity to be of the form

$$E_{\text{kin}} = \frac{e^2}{2a_B} (2a_B\beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) \quad (\text{III.52})$$

$(a_B \doteq \frac{\hbar^2}{Me^2} \dots \text{Bohr radius})$

with the kinetic function $\varepsilon_{\text{kin}}(\nu)$ being given by

$$\varepsilon_{\text{kin}}(\nu) = \frac{1}{2\nu+1} \left(\frac{1}{4} + \frac{l_\varphi^2}{2\nu} \right). \quad (\text{III.53})$$

- (ii) Solve the Poisson equation (III.36) for the spherically symmetric potential ${}^{[p]}A_0(r)$ (**App.A**) and compute by means of this result the electrostatic gauge field energy $E_R^{[e]}$ (III.45) which then emerges as follows

$$E_R^{[e]} = -\frac{e^2}{a_B} (2\beta a_B) \cdot \varepsilon_{\text{pot}}(\nu) . \quad (\text{III.54})$$

Here the potential function $\varepsilon_{\text{pot}}(\nu)$ may be expressed in two alternative ways on account of the Poisson identity (III.47), see equation (A.28) of **App.A**. (For a sketch of the spherically symmetric trial potentials ${}^{[p]}A_0(r)$ (III.37), see **Fig.A.I**).

- (iii) Substituting both energy contributions E_{kin} (III.52) and $E_R^{[e]}$ (III.54) back into the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) yields a certain function $\mathbb{E}^{(IV)}(\beta, \nu)$ of the two variational parameters β and ν , see equation (A.22) of **App.A**:

$$\mathbb{E}^{(IV)}(\beta, \nu) = \frac{e^2}{a_B} \left\{ (2a_B\beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (2a_B\beta) \cdot \varepsilon_{\text{pot}}(\nu) \right\} . \quad (\text{III.55})$$

(Observe here that both the normalization condition (III.46) for the wave amplitude $\tilde{\Phi}(r)$ and the Poisson identity (III.47) are satisfied, so that the energy function $\mathbb{E}^{(IV)}(\beta, \nu)$ due to $\tilde{\mathbb{E}}_{[T]}$ (III.41) consists solely of the kinetic energy and the gauge field energy).

- (iv) The extremalization process (III.40) can now be carried through for the obtained function $\mathbb{E}^{(IV)}(\beta, \nu)$ (III.55). Here it is most convenient to perform this in two steps: After the extremalization with respect to β (cf. (A.23a)), there remains to look for the minimal values ($\mathbb{E}_T(\nu_*)$, say) of the reduced energy function $\mathbb{E}_T(\nu)$

$$\mathbb{E}_T(\nu) \doteq -\frac{e^2}{4a_B} \cdot S_\varphi(\nu) \quad (\text{III.56a})$$

$$S_\varphi(\nu) \doteq \frac{\varepsilon_{\text{pot}}^2(\nu)}{\varepsilon_{\text{kin}}(\nu)} . \quad (\text{III.56b})$$

Such a minimization process may be achieved by means of an appropriate computer program. The conventional predictions (I.4) would be obtained if the *spectral*

function $S_\wp(\nu)$ took its maximal values at

$$S_\wp \Big|_{\max} \Rightarrow \frac{1}{n_\wp^2} . \quad (\text{III.57})$$

$$(n_\wp = 1, 2, 3, \dots)$$

Of course, this dream result cannot be attained by use of such a simple trial amplitude as the selected $\tilde{\Phi}(r)$ (III.50); but nevertheless the present approximation procedure yields predictions $\mathbb{E}_T(\nu_*)$ which come amazingly close to the conventional predictions $E_{\text{conv}}^{(n)}$ (I.4), see the subsequent **table 1**.

n_φ ($= l_\varphi + 1$)	$E_{\text{conv}}^{(n)}$ [eV], (I.4)	$\mathbb{E}_T(\nu_*^{[n]})$ [eV], (III.56a)	$\nu_*^{[n]}$	$\frac{E_{\text{conv}}^{(n)} - \mathbb{E}_T(\nu_*^{[n]})}{E_{\text{conv}}^{(n)}} [\%]$
1	-6.80290 ...	-7.23055 ...	-0.2049	-6.3
2	-1.70072 ...	-1.55087 ...	1.7942	8.8
3	-0.75588 ...	-0.66914 ...	3.7528	11.5
4	-0.42518 ...	-0.37366 ...	5.8740	12.1
5	-0.27212 ...	-0.23906 ...	8.1307	12.1
6	-0.18897 ...	-0.16637 ...	10.5044	12.0
10	-0.06803 ...	-0.06069 ...	20.9538	10.8
15	-0.03024 ...	-0.02735 ...	35.7017	9.5
20	-0.01701 ...	-0.01555 ...	51.9196	8.6
25	-0.01088 ...	-0.01003 ...	69.3583	7.9
30	-0.00756 ...	-0.00701 ...	87.8627	7.3
35	-0.00555 ...	-0.00518 ...	107.3506	6.8
40	-0.00425 ...	-0.00398 ...	127.8215	6.4
45	-0.00336 ...	-0.00316 ...	149.3660	6.1
50	-0.00272 ...	-0.00256 ...	172.1617	5.8
60	-0.00189 ...	-0.00179 ...	222.5187	5.3
70	-0.00139 ...	-0.00132 ...	280.9499	4.8
80	-0.00106 ...	-0.00102 ...	348.2861	4.5
90	-0.00084 ...	-0.00081 ...	422.8567	4.1
100	-0.00068 ...	-0.00065 ...	501.4648	3.8

Table 1: *Conventional Predictions and Spherically Symmetric Approximation*

The minimization of the RST energy function $\mathbb{E}_T(\nu)$ (III.56a)-(III.56b) with respect to the second variational parameter ν occurs at the values $\nu_*^{[n]}$ (fourth column) and yields the corresponding RST prediction $\mathbb{E}_T(\nu_*^{[n]})$ (third column). The relative deviation from

the conventional prediction $E_{\text{conv}}^{(n)}$ (I.4) is displayed in the last column; this deviation decreases from (roughly) 10% at low quantum numbers $n_\phi \lesssim 10$ up to 4% for high quantum numbers ($n_\phi \sim 100$). Such a decrease of the relative deviation is necessary in order that no cross-over with the conventional predictions $E_{\text{conv}}^{(n)}$ can occur (see **Fig.III.A**). The negative deviation of the groundstate ($n_\phi = 1$, first line) is presumably caused by the weak singularity of the trial amplitude $\tilde{\Phi}(r)$ [11] (here $\nu_* = -0, 204\dots$, see **Fig.4b** of ref. [11]). Such a singularity signals a certain crowding of the electric charge in the vicinity of the origin ($r = 0$) with a non-zero Dirac current \vec{k}_p on the z-axis, see both **Fig.1** and equation (VI.30) in ref. [11]. Consequently, *magnetism* may not be neglected for this situation very close to the origin, and the presently used *electrostatic* approximation is assumed to break down for the groundstate ($n_\phi = 1$) from this reason. On the other hand, the excited states ($n_\phi > 1$) have vanishing Dirac current on the z-axis so that no magnetic excess force can occur and the electrostatic approximation allows for sufficiently realistic predictions.

The average deviation ($\overline{\Delta_{[T]}}$, say) due to the presently considered lowest order of the spherically symmetric approximation may be defined through

$$\overline{\Delta_{[T]}} \doteq \frac{1}{20} \sum_{n_\phi}^{100} |\Delta_T(\nu_*^{[n]})| , \quad (\text{III.58})$$

where the individual deviations $\Delta_T(\nu_*^{[n]})$ are specified by the last column of table 1, i.e.:

$$\Delta_T(\nu_*^{[n]}) \doteq \frac{E_{\text{conv}}^{(n)} - \mathbb{E}_T(\nu_*^{[n]})}{E_{\text{conv}}^{(n)}} . \quad (\text{III.59})$$

Thus the average deviation of the present predictions is found as $\overline{\Delta_{[T]}} = 7,7\%$. This will become halved through regarding the anisotropic corrections (**Sect.V**).

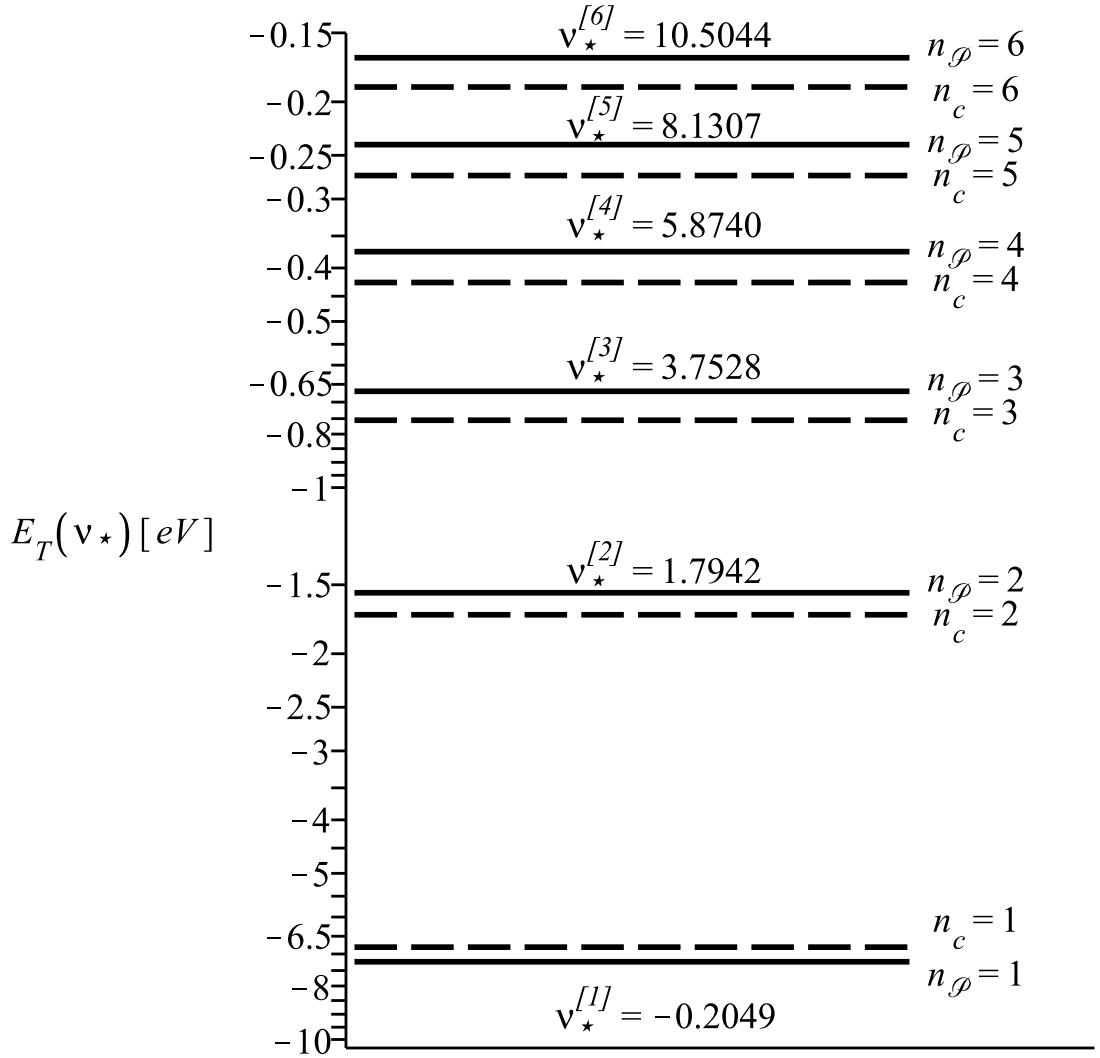


Fig. III.A Energy Spectrum in the Spherically Symmetric Approximation

The minimal values $\mathbb{E}_T(v_*^{[n]})$ (\rightsquigarrow solid lines) of the energy function $\mathbb{E}_T(\nu)$ (III.56a) are always unambiguously related to the corresponding conventional predictions $E_{\text{conv}}^{(n)}$ (I.4) (broken lines) because the relative deviations do not amount to more than (roughly) 10%, see also **table 1** on p. 44. Therefore there occurs no crossing-over of the conventional and

RST predictions which should provide a solid basis for estimating the magnitude of the anisotropic corrections in **Sect. IV**. The latter naïve type of corrections turns out to be of the order of (roughly) 0.4% for the groundstate, see equations (IV.45)-(IV.46) below, but would deteriorate the present “isotropic” RST predictions by (roughly) 8% already for the first excited state, see **App.C**. These unrealistic *large* anisotropy corrections for the *excited* states necessitates then a reconsideration and improvement of the applied approximation method (**Sect. V**).

IV Anisotropic Corrections of Gauge Potential

The necessity to go beyond the spherically symmetric approximation has already been stressed in the introduction (**Sect. I**). But in view of the preceding difficulties with obtaining exact solutions of the spherically symmetric type one will not expect that *anisotropic exact* solutions could ever be found. On the other hand, an estimate of the magnitude of the anisotropic effects would be highly desirable and we will try to attain this now at least partially, namely by expanding the formal solution (II.30) for the electrostatic potential ${}^{(p)}A_0(\vec{r})$ with respect to the longitudinal variable ϑ of the spherical polar coordinates (r, ϑ, ϕ) . This means that we relax the spherically symmetric approximation (III.1) to the following weaker condition:

$${}^{(p)}A_0(\vec{r}) \Rightarrow {}^{\{p\}}A_0(r, \vartheta). \quad (\text{IV.1})$$

Here the ϑ -dependent potential ${}^{\{p\}}A_0(r, \vartheta)$ needs not be the *exact* value of the integral in (II.30) but we will be satisfied with some approximative value in lowest order due to a certain *expansion with respect to the anisotropy effect*.

In any case, the latter effect will not be fully taken into account since we still adopt that form of the wave amplitudes ${}^{(p)}\mathcal{R}_{\pm}$, ${}^{(p)}\mathcal{S}_{\pm}$ as it results from the combination of the transformations (III.13a)-(III.13b), (III.14a)-(III.14b), (III.17a)-(III.17b), (III.19)-(III.20) and (III.23a)-(III.23b), i. e. in the last end:

$${}^{(p)}\mathcal{R}_{\pm}(\vec{r}) \Rightarrow \frac{\tilde{\Phi}_{\pm}(r) \cdot f_R(\vartheta)}{\sqrt{r \sin \vartheta}} \quad (\text{IV.2a})$$

$${}^{(p)}\mathcal{S}_{\pm}(\vec{r}) \Rightarrow \frac{\tilde{\Phi}_{\pm}(r) \cdot f_S(\vartheta)}{\sqrt{r \sin \vartheta}}. \quad (\text{IV.2b})$$

Observing here the solutions (III.19)-(III.20) for the angular functions $f_R(\vartheta)$ and $f_S(\vartheta)$, one finds for the Dirac density ${}^{(p)}k_0(\vec{r})$ (II.19)

$${}^{(p)}k_0(\vec{r}) \Rightarrow {}^{\{p\}}k_0(r, \vartheta) = \frac{\tilde{\Phi}_+^2(r) + \tilde{\Phi}_-^2(r)}{4\pi r \sin \vartheta}. \quad (\text{IV.3})$$

If this result is substituted into equation (II.30), the electrostatic potential ${}^{(p)}A_0(\vec{r})$ reappears.

pears as $\{^p\}A_0(r, \vartheta)$ in the following form

$$\{^p\}A_0(r, \vartheta) = \alpha_s \int \frac{d^3\vec{r}'}{4\pi r' \sin \vartheta'} \frac{\tilde{\Phi}_+^2(r') + \tilde{\Phi}_-^2(r')}{\|\vec{r} - \vec{r}'\|}, \quad (\text{IV.4})$$

or in the non-relativistic approximation ($\tilde{\Phi}_+(r) \Rightarrow \tilde{\Phi}(r)$, $\tilde{\Phi}_-(r) \Rightarrow 0$)

$$\{^p\}A_0(r, \vartheta) = \frac{\alpha_s}{4\pi} \int \frac{d^3\vec{r}'}{r' \sin \vartheta'} \frac{\tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|}. \quad (\text{IV.5})$$

From here it is seen that the anisotropy of the *wave amplitudes* themselves is taken into account only to that extent as it is assumed also in the spherically symmetric approximation for the potential $[^p]A_0(r)$ (III.37)! Thus, the main anisotropic effect is thought to be due to the formal modification of the three-volume element in equation (IV.5)

$$d^3\vec{r} \Rightarrow \frac{d^3\vec{r}}{r \sin \vartheta} = r dr d\vartheta d\phi, \quad (\text{IV.6})$$

where the denominator is a consequence of the former transformation (III.14a)-(III.14b) of the wave amplitudes. Accordingly, our step beyond the spherically symmetric approximation consists now in computing the potential $\{^p\}A_0(r, \vartheta)$

$$\{^p\}A_0(r, \vartheta) = \frac{\alpha_s}{4\pi} \int dr' d\vartheta' d\phi' \frac{\vec{r}' \cdot \tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|} \quad (\text{IV.7})$$

in an approximate way (i.e. in lowest order beyond the spherically symmetric approximation (III.1)) and then using the result for calculating the value of the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) on the present trial configuration $\{\tilde{\Phi}(r), \{^p\}A_0(r, \vartheta)\}$. The corresponding extremal values of $\tilde{\mathbb{E}}_{[\Phi]}$ within this class of trial configurations do then determine again the approximative RST energy levels of the bound system which must be opposed to both the conventional predictions and to the spherically symmetric RST predictions of **Sect. III.** Anticipating the result of this comparison, we will find that these anisotropy corrections are lowering the groundstate energy (first line of table 1 on p. 44) by 0.4% so that the anisotropy correction appears to be actually a negligible perturbation of the spherical symmetry. However, this pleasant result is readily shown to hold only for the groundstate

(App.B) and even here is spurious so that we are forced to develeop a more realistic perturbation procedure (Sect.V).

1. Anisotropic Potentials

The wanted method of expanding the electrostatic potential $\{^p\}A_0(r, \vartheta)$ (IV.7) with respect to the magnitude of anisotropy will (in the simplest case) consist in naïvely expanding the denominator as follows:

$$\begin{aligned}\frac{1}{\|\vec{r} - \vec{r}'\|} &= \frac{1}{(r^2 + r'^2)^{\frac{1}{2}}} + \frac{rr'}{(r^2 + r'^2)^{\frac{3}{2}}} (\hat{\vec{r}} \cdot \hat{\vec{r}'}) + \frac{3}{2} \frac{r^2 r'^2}{(r^2 + r'^2)^{\frac{5}{2}}} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^2 \\ &+ \frac{5}{2} \frac{r^3 r'^3}{(r^2 + r'^2)^{\frac{7}{2}}} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^3 + \frac{35}{8} \frac{r^4 r'^4}{(r^2 + r'^2)^{\frac{9}{2}}} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^4 + \dots\end{aligned}\quad (\text{IV.8})$$

$$(\hat{\vec{r}} \doteq \frac{\vec{r}}{\|\vec{r}\|} = \frac{\vec{r}}{r} \Rightarrow \|\hat{\vec{r}}\|^2 = \|\hat{\vec{r}'}\|^2 = 1) .$$

Obviously, such a naïve expansion would induce a corresponding expansion of the potential $\{^p\}A_0(r, \vartheta)$ of the following product type:

$$\begin{aligned}\{^p\}A_0(r, \vartheta) &= \{^p\}A_I(\vartheta) \cdot \{^p\}A_I(r) + \{^p\}A_{II}(\vartheta) \cdot \{^p\}A_{II}(r) + \{^p\}A_{III}(\vartheta) \cdot \{^p\}A_{III}(r) \\ &+ \{^p\}A_{IV}(\vartheta) \cdot \{^p\}A_{IV}(r) + \{^p\}A_V(\vartheta) \cdot \{^p\}A_V(r) + \dots\end{aligned}\quad (\text{IV.9})$$

Here, the angular factors are found to look as follows

$$\{^p\}A_I(\vartheta) \doteq \int \frac{d\vartheta' d\phi'}{4\pi} = \frac{\pi}{2} \quad (\text{IV.10a})$$

$$\{^p\}A_{II}(\vartheta) \doteq \int \frac{d\vartheta' d\phi'}{4\pi} (\hat{\vec{r}} \cdot \hat{\vec{r}'}) = 0 \quad (\text{IV.10b})$$

$$\{^p\}A_{III}(\vartheta) \doteq \frac{3}{2} \int \frac{d\vartheta' d\phi'}{4\pi} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^2 = \frac{3}{16} \pi (1 + \cos^2 \vartheta) \quad (\text{IV.10c})$$

$$\{^p\}A_{IV}(\vartheta) \doteq \frac{5}{2} \int \frac{d\vartheta' d\phi'}{4\pi} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^3 = 0 \quad (\text{IV.10d})$$

$$\{^p\}A_V(\vartheta) \doteq \frac{35}{8} \int \frac{d\vartheta' d\phi'}{4\pi} (\hat{\vec{r}} \cdot \hat{\vec{r}'})^4 = \frac{105}{128} \pi \{ \cos^4 \vartheta + \cos^2 \vartheta \sin^2 \vartheta + \frac{3}{8} \sin^4 \vartheta \} \quad (\text{IV.10e})$$

⋮

Evidently, these angular factors do not display the expected tendency of decreasing with increasing order of the expansion terms; therefore such a decreasing tendency must arise now with the radial factors, otherwise the series expansion (IV.9) of the potential $\{^p\}A_0(r, \vartheta)$ would not be convergent.

The radial factors emerging in the expansion (IV.9) are found to look as follows:

$$\{^p\}A_I(r) = \alpha_s \cdot \int_0^\infty dr' \frac{r' \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{1}{2}}} \quad (\text{IV.11a})$$

$$\{^p\}A_{II}(r) = \alpha_s \cdot r \int_0^\infty dr' \frac{r'^2 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{3}{2}}} \quad (\text{IV.11b})$$

$$\{^p\}A_{III}(r) = \alpha_s \cdot r^2 \int_0^\infty dr' \frac{r'^3 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{5}{2}}} \quad (\text{IV.11c})$$

$$\{^p\}A_{IV}(r) = \alpha_s \cdot r^3 \int_0^\infty dr' \frac{r'^4 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{7}{2}}} \quad (\text{IV.11d})$$

$$\{^p\}A_V(r) = \alpha_s \cdot r^4 \int_0^\infty dr' \frac{r'^5 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{9}{2}}} \quad (\text{IV.11e})$$

\vdots

Observe here that both potentials $\{^p\}A_{II}(r)$ (IV.11b) and $\{^p\}A_{IV}(r)$ (IV.11d) are irrelevant because they become eliminated by their vanishing angular pre-factors $\{^p\}A_{II}(\vartheta)$ (IV.10b) and $\{^p\}A_{IV}(\vartheta)$ (IV.10d). Concerning the relative magnitude of the remaining potentials $\{^p\}A_I(r)$ (IV.11a), $\{^p\}A_{III}(r)$ (IV.11c) and $\{^p\}A_V(r)$ (IV.11e) one could of course explicitly compute these potentials by resorting to the former trial amplitude $\tilde{\Phi}(r)$ (III.50) which then would immediately yield the desired relative magnitudes. However, one may circumvent those unwieldy integrals by establishing a certain differential link between these radial auxiliary potentials (IV.11a)-(IV.11e) and then adopt a plausible guess for the lowest-order potential $\{^p\}A_I(r)$. This guess can then be taken as the point of departure for calculating the higher-order potentials $\{^p\}A_{III}(r)$, $\{^p\}A_V(r)$, ... just by means of that established differential link (see below).

Concerning now the relative magnitude of the partial potentials $\{^p\}A_l(r, \vartheta) = \{^p\}A_l(\vartheta) \cdot \{^p\}A_l(r)$ etc., cf. (IV.9), it is obviously sufficient to consider their radial factors $\{^p\}A_l(r)$ etc., cf. (IV.11a)-(IV.11e). Here, the first one (i.e. $\{^p\}A_l(r)$ (IV.11a)) is singled out by its boundary values for $r = 0, \infty$. At the origin ($r = 0$) one finds

$$\{^p\}A_l(r)\Big|_{r=0} = \alpha_s \int_0^\infty dr' \tilde{\Phi}^2(r') , \quad (\text{IV.12})$$

i.e. for the spherically symmetric trial function $\tilde{\Phi}(r)$ (III.50)

$$\{^p\}A_l(r)\Big|_{r=0} \Rightarrow \frac{2}{\pi} (2\beta\alpha_s) \cdot \frac{1}{2\nu + 1} . \quad (\text{IV.13})$$

Combinig this with its angular associate $\{^p\}A_l(\vartheta)$ (IV.10a) yields then at the origin

$$\{^p\}A_l(r, \vartheta)\Big|_{r=0} = [\{^p\}A_l(\vartheta) \cdot \{^p\}A_l(r)]_{r=0} \Rightarrow \frac{2\beta\alpha_s}{2\nu + 1} , \quad (\text{IV.14})$$

which just agrees with the value of the spherically symmetric approximation $[^p]A_0(r)$ at the origin ($r = 0$), cf. the equation (A.10) of **App. A**. On the other hand, this value (IV.12) of the first auxiliary potential $\{^p\}A_l(r, \vartheta)$ (or its specialization (IV.14), resp.) at the origin ($r = 0$) actually coincides with the corresponding value of the “exact” solution $\{^p\}A_0(r, \vartheta)$ (IV.7):

$$\{^p\}A_0(r, \vartheta)\Big|_{r=0} = \frac{\alpha_s}{4\pi} \int dr' d\vartheta' d\phi' \tilde{\Phi}^2(r') = \frac{\pi}{2} \alpha_s \int_0^\infty dr' \tilde{\Phi}^2(r') \equiv \frac{\pi}{2} \cdot \{^p\}A_l(r = 0) , \quad (\text{IV.15})$$

see equation (IV.12). Thus the conclusion is now the following: since already the first auxiliary potential $\{^p\}A_l(r, \vartheta) = \{^p\}A_l(\vartheta) \cdot \{^p\}A_l(r)$ in the expansion (IV.9) for $\{^p\}A_0(r, \vartheta)$ adopts the correct value of $\{^p\}A_0(r, \vartheta)$ at the origin, all other auxiliary potentials must necessarily vanish at the origin ($r = 0$); or expressed in terms of the radial potentials (IV.11b)-(IV.11e)

$$\{^p\}A_{\text{III}}(r)\Big|_{r=0} = \{^p\}A_V(r)\Big|_{r=0} = \dots = 0 . \quad (\text{IV.16})$$

A similar conclusion does also hold for the behaviour of the radial auxiliary potentials at infinity ($r \rightarrow \infty$). First, observe here that the “exact” anisotropic solution (IV.7)

adopts the Coulomb form for $r \rightarrow \infty$

$$\lim_{r \rightarrow \infty} {}^{\{p\}}A_0(r, \vartheta) = \frac{\alpha_s}{r} \cdot \frac{\pi}{2} \int_0^\infty dr' r' \tilde{\Phi}^2(r') = \frac{\alpha_s}{r} , \quad (\text{IV.17})$$

provided the non-relativistic wave amplitude $\tilde{\Phi}(r)$ obeys the normalization condition (III.38). But on the other hand, the first-order radial potential ${}^{\{p\}}A_I(r)$ (IV.11a) has just the same limit form (apart from the angular factor (IV.10a)):

$$\lim_{r \rightarrow \infty} {}^{\{p\}}A_I(r) = \frac{2}{\pi} \cdot \frac{\alpha_s}{r} , \quad (\text{IV.18})$$

and therefore the expansion (IV.9) tells us that the higher-order potentials must vanish faster than $\frac{1}{r}$ at infinity:

$$\lim_{r \rightarrow \infty} {}^{\{p\}}A_{\text{III}}(r) = \lim_{r \rightarrow \infty} {}^{\{p\}}A_V(r) = \dots = \mathcal{O}\left(\frac{1}{r^2}\right) . \quad (\text{IV.19})$$

Since both the second potential ${}^{\{p\}}A_{\text{II}}(r)$ (IV.11b) and the fourth potential ${}^{\{p\}}A_{\text{IV}}(r)$ (IV.11d) become annihilated by their angular counterparts ${}^{\{p\}}A_{\text{II}}(\vartheta)$ (IV.10b) and ${}^{\{p\}}A_{\text{IV}}(\vartheta)$ (IV.10d), it is sufficient to look for the announced link only between the non-zero potentials ${}^{\{p\}}A_I(r)$ (IV.11a), ${}^{\{p\}}A_{\text{III}}(r)$ (IV.11c) and ${}^{\{p\}}A_V(r)$ (IV.11e). For this purpose, one differentiates twice the first potential ${}^{\{p\}}A_I(r)$ (IV.11a) and thereby finds immediately for the third potential ${}^{\{p\}}A_{\text{III}}(r)$ (IV.11c)

$${}^{\{p\}}A_{\text{III}}(r) = -\frac{1}{3} r \frac{d^2}{dr^2} [r \cdot {}^{\{p\}}A_I(r)] . \quad (\text{IV.20})$$

A similar procedure yields for the fifth potential ${}^{\{p\}}A_V(r)$ (IV.11e)

$${}^{\{p\}}A_V(r) = -\frac{1}{35} r^3 \frac{d}{dr} \left[\frac{1}{r^4} \frac{d}{dr} (r^3 \cdot {}^{\{p\}}A_{\text{III}}(r)) \right] , \quad (\text{IV.21})$$

etc. The importance of this procedure is now that one can guess some reasonable approximation for the lowest-order potential ${}^{\{p\}}A_I(r)$ which is manageable more conveniently than the integral on the right-hand side of equation (IV.11a) but which on the other hand comes sufficiently close to the value of that integral. If this guess for ${}^{\{p\}}A_I(r)$ is substituted in equation (IV.20), one obtains the corresponding approximative expressions for

the higher-order potentials $\{^p\}A_{\text{III}}(r)$ and $\{^p\}A_{\text{V}}(r)$ whose relative magnitude can then be estimated.

2. Simplified Groundstate Potentials ($\nu = 0$)

For the purpose of a simple demonstration of our approximation method, a *preliminary* choice for the lowest-order potential $\{^p\}A_1(r)$ could perhaps consist in the spherically symmetric potential $[^p]A_0(r)$ ((A.2) plus (A.5) for $\nu = 0$) which has been treated extensively in the precedent **Sect. III** (and also in **App. A**, where the trial amplitude $\tilde{\Phi}(r)$ (III.50) does underlie). Deferring again the purely technical subtleties to **App. C**, we can be satisfied here for the sake of demonstration with the special case $\nu = 0$ where the selected trial amplitude $\tilde{\Phi}(r)$ (III.50) becomes especially simple because there remains only one variational parameter (β):

$$\tilde{\Phi}(r) \Rightarrow \Phi_* e^{-\beta r} \quad (\text{IV.22a})$$

$$\Phi_* = \sqrt{\frac{2}{\pi}} (2\beta) . \quad (\text{IV.22b})$$

The corresponding spherically symmetric solution $[^p]A_0(r)$ of the Poisson equation (III.36) looks as follows:

$$[^p]A_0(r) = \frac{\alpha_s}{r} (1 - e^{-2\beta r}) . \quad (\text{IV.23})$$

Thus the asymptotic Coulomb form (IV.18) of the first auxiliary potential $\{^p\}A_1(r, \vartheta)$ is safely adopted by the present spherically symmetric approximation (IV.23). Furthermore, the value of the “exact” anisotropic solution $\{^p\}A_0(r, \vartheta)$ (IV.7) at the origin

$$\{^p\}A_0(r, \vartheta) \Big|_{r=0} = \alpha_s \frac{\pi}{2} \int_0^\infty dr' \tilde{\Phi}^2(r') = 2\beta\alpha_s \quad (\text{IV.24})$$

also does agree with the corresponding value of that spherically symmetric approximation $[^p]A_0(r)$ (IV.23). Summarizing, the boundary values of the “exact” anisotropic potential $\{^p\}A_0(r, \vartheta)$ (IV.7) are truly reproduced by the present spherically symmetric candidate

$[^p]A_0(r)$ (IV.23); and this justifies to *preliminarily* adopt just that potential $[^p]A_0(r)$ as the starting point for generating the series of higher-order approximations via the differential link (IV.20)-(IV.21), i. e. we try

$$\{^p\}A_I(r) \Rightarrow \frac{2}{\pi} \cdot [^p]A_0(r) = \frac{2}{\pi} \frac{\alpha_s}{r} (1 - e^{-2\beta r}) . \quad (\text{IV.25})$$

But once such a convention concerning the starting potential $\{^p\}A_I(r)$ has been attained, one can now substitute this into the differential links (IV.20)-(IV.21) in order to calculate the higher-order potentials $\{^p\}A_{III}(r)$ and $\{^p\}A_V(r)$, etc. Indeed, by this simple process of differentiation one easily finds the following results

$$\{^p\}A_{III}(r) \Rightarrow \frac{8}{3\pi} \alpha_s \beta^2 r e^{-2\beta r} \quad (\text{IV.26a})$$

$$\{^p\}A_V(r) \Rightarrow -\frac{16}{105\pi} (2\beta\alpha_s) e^{-2\beta r} \left\{ \frac{(2\beta r)^3}{8} - \frac{1}{2} (2\beta r)^2 - \frac{1}{2} (2\beta r) \right\} . \quad (\text{IV.26b})$$

Fig.IV.A below presents a sketch of all three radial potentials $\{^p\}A_I(r)$ (IV.25), $\{^p\}A_{III}(r)$ (IV.26a) and $\{^p\}A_V(r)$ (IV.26b) which clearly shows the hierarchy of their magnitudes. Thus it is evident that the expansion (IV.9) of the anisotropic potential $\{^p\}A_0(r, \vartheta)$ yields a (more or less rapidly) converging series of radial auxiliary potentials (IV.11a) etc. which constitutes a kind of “*expansion with respect to the magnitude of anisotropy*”. For general variational parameter ν , this effect is studied in **App.B**. The result is that for all values of the variational parameter $\nu (> -\frac{1}{2})$ the magnitude of the radial potentials $\{^p\}A_I(r)$, $\{^p\}A_{III}(r)$, $\{^p\}A_V(r)$, ... is decreasing rapidly enough (see **Fig.B.I**) in order that one can tentatively restrict oneself to the first anisotropic contribution $\{^p\}A_{III}(r, \vartheta)$ for an estimate of the anisotropic effect upon the energy \mathbb{E}_T which is concentrated in those anisotropic field configurations.

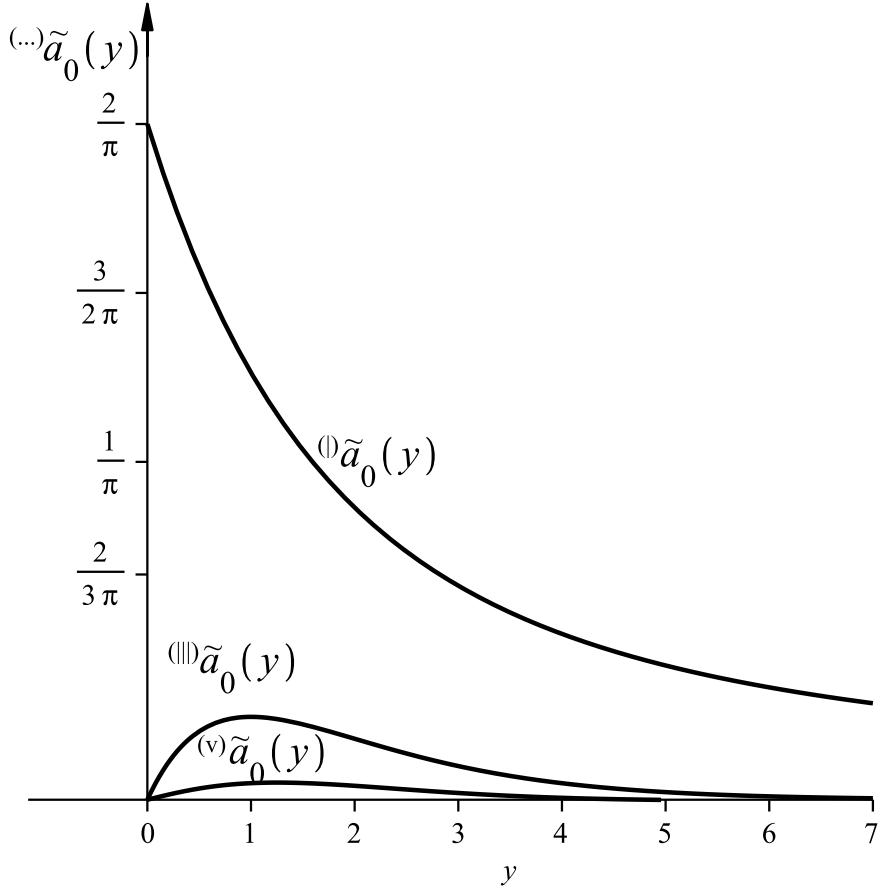


Fig. IV.A Radial Auxiliary Potentials $\{^p\}A_I$, $\{^p\}A_{III}$, $\{^p\}A_V$

The potentials (IV.25)-(IV.26b) for $\nu = 0$ are sketched in dimensionsless units, cf. equations (B.6)-(B.10) of **App. B**. For the present case $\nu = 0$ there is a distinct hierarchy of magnitudes ($\{^V\}\tilde{a}_0 < \{^{III}\}\tilde{a}_0 < \{^0\}\tilde{a}_0$) which lets the anisotropy corrections for the simplified groundstate ($\nu = 0$) appear as small as only 0.4% (see the discussion below equation (IV.43)). For the excited states ($\nu > 0$), this hierarchy of magnitudes becomes flattened (see **Fig.B.I** on page 108) and consequently the anisotropy corrections of the excited states do amount up to some unrealistic 10% and more, even for the first excited state (see the table on page 114) which necessitates to set up a more adequate series expansion than given by equations (IV.9)-(IV.11e), see **Sect.V**.

3. Energy of the Simplified Anisotropic Groundstate ($\nu = 0$)

After a choice of some trial amplitude $\tilde{\Phi}(r)$ (III.50) has been made together with the subsequent determination of the corresponding anisotropic potential $\{^p\}A_0(r, \vartheta)$ (IV.7) (to be used only up to a certain order of approximation) one can now tackle more concretely the problem of the total energy E_T which is carried by such an anisotropic configuration. Here it may be sufficient (for a first rough estimate of the anisotropy effect) to restrict oneself to the inclusion of only the *first* anisotropic correction term $\{^p\}A_{\text{III}}(r, \vartheta) = \{^p\}A_{\text{III}}(\vartheta) \cdot \{^p\}A_{\text{III}}(r)$. By this restriction, one can represent the general approximation method in a rather transparent way without the numerical calculations becoming too tedious. But observe here that we have to admit a certain complication which consists in the fact that our adopted approximative potential (cf. (IV.9))

$$\{^p\}A_0(r, \vartheta) \Rightarrow \{^p\}A_{\text{I}}(r, \vartheta) + \{^p\}A_{\text{III}}(r, \vartheta) = \{^p\}A_{\text{I}}(\vartheta) \cdot \{^p\}A_{\text{I}}(r) + \{^p\}A_{\text{III}}(\vartheta) \cdot \{^p\}A_{\text{III}}(r) \quad (\text{IV.27})$$

is *not* an exact solution of the non-relativistic Poisson equation

$$\Delta \{^p\}A_0(r, \vartheta) = -\alpha_s \frac{\tilde{\Phi}^2(r)}{r \sin \vartheta}, \quad (\text{IV.28})$$

i. e. the non-relativistic version of (III.16). As a consequence, the non-relativistic Poisson identity $\tilde{N}_G^{(e)} \equiv 0$ (II.35) will not be satisfied, in contrast to the normalization condition $\tilde{N}_{\Phi} \equiv 0$ (III.46) which merely fixes the normalization constant Φ_* (see equation (III.51)). Therefore the energy functional $\tilde{E}_{[\Phi]}$ (III.41) does not reduce to its proper physical part $E_{[\Phi]}^{(\text{IV})}$ ($\doteq 2E_{\text{kin}} + E_R^{(e)}$) but must be kept somewhat more general:

$$\tilde{E}_{[\Phi]} \Rightarrow 2E_{\text{kin}} + E_R^{(e)} + \lambda_G^{(e)} \cdot \tilde{N}_G^{(e)}. \quad (\text{IV.29})$$

Thus the problem is now to look for the value of this functional on the class of trial configurations for the groundstate which by assumption is parametrized by only one variational parameter β (because of putting $\nu = 0$). This will yield a function $\tilde{E}_{\Phi}(\beta)$ whose minimal value is just the desired total energy ($E_T^{(1)}$, say) of the anisotropic groundstate;

and the crucial questions with this result are now **(i)** how close is this RST prediction $\mathbb{E}_T^{\{1\}}$ to the corresponding conventional prediction $E_{\text{conv}}^{(1)}$ (I.4), and **(ii)** how large is the *anisotropic* contribution (beyond the spherically symmetric approximation) included in this RST prediction $\mathbb{E}_T^{\{1\}}$?

For working through this program, one evokes the trial amplitude $\tilde{\Phi}(r)$ for the ground-state (IV.22a)-(IV.22b) in combination with the associated (but approximative) gauge potential $\{^p\}A_0(r, \vartheta)$ (IV.27), with the angular parts $\{^p\}A_l(\vartheta)$ and $\{^p\}A_{lll}(\vartheta)$ given by equations (IV.10a) and (IV.10c) and the radial parts $\{^p\}A_l(r)$ and $\{^p\}A_{lll}(r)$ being given by (IV.25) and (IV.26a); i. e. the (one-parametric) trial potential due to the (one-parametric) trial amplitude $\tilde{\Phi}(r)$ (IV.22a) reads ultimately

$$\{^p\}A_0(r, \vartheta) \Rightarrow \frac{\pi}{2} \cdot \frac{2 \alpha_s}{\pi r} (1 - e^{-2\beta r}) + \frac{3}{16} \pi (1 + \cos^2 \vartheta) \cdot \frac{8}{3\pi} \alpha_s \beta^2 r e^{-2\beta r}. \quad (\text{IV.30})$$

Both these trial ansätze $\tilde{\Phi}(r)$ (IV.22a) and $\{^p\}A_0(r, \vartheta)$ (IV.30) are now to be used in order to calculate any individual contribution to the energy function $\tilde{\mathbb{E}}_\Phi(\beta)$ as the value of the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (IV.29) on this trial configuration.

The first contribution is the kinetic energy E_{kin} (III.42) which itself is the sum of the radial part ${}^{(r)}E_{\text{kin}}$ (III.43) and the longitudinal part ${}^{(\vartheta)}E_{\text{kin}}$ (III.44). The latter, however, must vanish for the groundstate because here we assume the quantum number l_ϑ of angular momentum (III.21) to be zero ($\Rightarrow l_\vartheta = 0$). Thus the (one-particle) kinetic energy is of purely radial nature, cf. (III.52)-(III.53) for $l_\vartheta = 0$ and $\nu = 0$

$$E_{\text{kin}} \Rightarrow {}^{(r)}E_{\text{kin}} = \frac{\hbar^2}{2M} \cdot \frac{\pi}{2} \int_0^\infty dr r \left(\frac{d\tilde{\Phi}(r)}{dr} \right)^2 = \frac{e^2}{2a_B} (\beta a_B)^2 \quad (\text{IV.31})$$

$$(a_B = \frac{\hbar^2}{Me^2} \dots \text{Bohr radius}).$$

The next energy contribution is the electrostatic gauge field energy $E_R^{(e)}$ (II.36) which reads in terms of our anisotropic potential $\{^p\}A_0(r, \vartheta)$ (IV.30)

$$E_R^{(e)} \Rightarrow E_R^{\{e\}} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3\vec{r} \|\vec{\nabla} \{^p\}A_0(r, \vartheta)\|^2 \doteq E_l^{\{e\}} + E_{ll}^{\{e\}} + E_{lll}^{\{e\}}, \quad (\text{IV.32})$$

with the three contributions being found by explicit integration as (cf. **App. C**)

$$E_{\text{I}}^{\{e\}} = -\hbar c \alpha_s \beta = -e^2 \beta \quad (\text{IV.33a})$$

$$E_{\text{II}}^{\{e\}} = -\frac{1}{6} \hbar c \alpha_s \beta = -\frac{1}{6} e^2 \beta \quad (\text{IV.33b})$$

$$E_{\text{III}}^{\{e\}} = -\frac{3}{160} \hbar c \alpha_s \beta = -\frac{3}{160} e^2 \beta . \quad (\text{IV.33c})$$

Here, the first contribution $E_{\text{I}}^{\{e\}}$ (IV.33a) is due to the spherically symmetric constituent $\{p\}A_{\text{I}}(r, \vartheta)$ ($= \{p\}A_{\text{I}}(\vartheta) \cdot \{p\}A_{\text{I}}(r)$) of the potential (IV.9) with the angular part $\{p\}A_{\text{I}}(\vartheta)$ being given by (IV.10a) and the radial part $\{p\}A_{\text{I}}(r)$ by the postulate (IV.25). Therefore the first expansion term $\{p\}A_{\text{I}}(r, \vartheta)$ just coincides with the spherically symmetric approximation $[p]A_0(r)$. Consequently, the present first contribution $E_{\text{I}}^{\{e\}}$ (IV.33a) must be identical to the field energy $E_{\text{R}}^{[e]}$ (III.54) of the spherically symmetric approximation, i. e. we must find for the sake of consistency:

$$E_{\text{I}}^{\{e\}} = -e^2 \beta \stackrel{!}{=} -2\beta e^2 \cdot \varepsilon_{\text{pot}}(0) \equiv E_{\text{R}}^{[e]} . \quad (\text{IV.34})$$

However, this consistency requirement

$$2 \cdot \varepsilon_{\text{pot}}(0) = 1 \quad (\text{IV.35})$$

is easily validated, namely simply by specializing the general result (A.28) of **App. A** down to $\nu = 0$ which yields

$$\varepsilon_{\text{pot}}(0) = 1 - \frac{1}{4} \cdot \sum_{n=0}^{\infty} \frac{n}{2^n} = \frac{1}{2} . \quad (\text{IV.36})$$

But whilst the first contribution $E_{\text{I}}^{\{e\}}$ (IV.33a) does refer to the spherically symmetric approximation, the other two contributions $E_{\text{II}}^{\{e\}}$ and $E_{\text{III}}^{\{e\}}$ (IV.33b)-(IV.33c) must represent the *anisotropic correction* ($E_{\text{a}}^{\{e\}}$, say)

$$E_{\text{a}}^{\{e\}} \doteq E_{\text{II}}^{\{e\}} + E_{\text{III}}^{\{e\}} = -\left(\frac{1}{6} + \frac{3}{160}\right) e^2 \beta = -\frac{89}{480} e^2 \beta . \quad (\text{IV.37})$$

However, the point with this anisotropic correction $E_{\text{a}}^{\{e\}}$ (IV.37) is now that it obviously cannot be considered as a *negligibly small* correction of the spherically symmetric term

$E_l^{\{e\}}$ (IV.34)! Thus the problem arises now how it may come about that the anisotropy corrections can be effectively smaller than the spherically symmetric contribution $E_l^{\{e\}}$ (IV.34)! Otherwise one could in general not consider $E_l^{\{e\}}$ as the leading term of a meaningful perturbation expansion. Indeed, we will readily show that this effect is based upon a certain peculiarity of the *principle of minimal energy*.

This question concerns now the last term of the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ on the right-hand side of equation (IV.29). Namely, this contribution is non-zero whenever the Poisson equation is not satisfied by the selected trial configuration, i. e. more precisely: whenever the trial configuration $\{\{^p\}A_0(r, \vartheta), \tilde{\Phi}(r)\}$ does not obey the Poisson equation (IV.28) for the gauge potential $\{^p\}A_0(r, \vartheta)$. Since our selected approximation (IV.27) for $\{^p\}A_0(r, \vartheta)$ contains only the first two non-vanishing terms of the general expansion (IV.9), it is not linked to the chosen trial amplitude $\tilde{\Phi}(r)$ (IV.22a)-(IV.22b) via the Poisson equation (IV.28); and therefore the anisotropic Poisson constraint (II.35) is violated. This then necessitates to explicitly calculate the constraint term $\tilde{\mathbb{N}}_G^{(e)}$

$$\mathbb{N}_G^{(e)} \Rightarrow \tilde{\mathbb{N}}_G^{(e)} = E_R^{\{e\}} - \tilde{\mathbb{M}}^{\{e\}} c^2 \quad (\text{IV.38})$$

which enters the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (IV.29) as the last term on the right-hand side.

Here, the gauge field energy $E_R^{\{e\}}$ has already been determined by equations (IV.32)-(IV.33c) so that we are left with the calculation of the (non-relativistic) mass equivalent $\tilde{\mathbb{M}}^{\{e\}} c^2$ (II.37). If our approximative potential $\{^p\}A_0(r, \vartheta)$ (IV.27), i. e. more precisely (IV.30) for the present groundstate situation, is substituted therein, one finds that the mass equivalent appears as a sum of two terms

$$\mathbb{M}^{\{e\}} c^2 \Rightarrow \tilde{\mathbb{M}}^{\{e\}} c^2 = \tilde{\mathbb{M}}_I^{\{e\}} c^2 + \tilde{\mathbb{M}}_{III}^{\{e\}} c^2 , \quad (\text{IV.39})$$

where the first term contains the spherically symmetric approximation $\{^p\}A_I(r)$ (IV.25) of the potential $\{^p\}A_0(r, \vartheta)$ and yields the following result

$$\tilde{\mathbb{M}}_I^{\{e\}} c^2 = - \left(\frac{\pi}{2}\right)^2 \hbar c \int_0^\infty dr r \cdot \{^p\}A_I(r) \cdot \tilde{\Phi}^2(r) = -\hbar c \alpha_s \beta \equiv E_I^{\{e\}} , \quad (\text{IV.40})$$

cf. (IV.34); and furthermore the second contribution is due to the first anisotropic correction (IV.26a) of $\{^p\}A_0(r, \vartheta)$:

$$\tilde{\mathbb{M}}_{\text{III}}^{\{e\}} c^2 = - \left(\frac{3\pi}{8} \right)^2 \hbar c \int_0^\infty dr r \{^p\}A_{\text{III}}(r) \cdot \tilde{\Phi}^2(r) = - \frac{3}{32} \hbar c \alpha_s \beta . \quad (\text{IV.41})$$

(For both results (IV.40) and (IV.41) the angular parts of the potentials are already integrated over). It should not come as a surprise that the lowest-order mass equivalent $\tilde{\mathbb{M}}_{\text{I}}^{\{e\}} c^2$ (IV.40) exactly agrees with the first contribution $E_{\text{I}}^{\{e\}}$ (IV.33a) to the gauge field energy $E_{\text{R}}^{\{e\}}$ (IV.32)! The reason for this is of course that both quantities $E_{\text{I}}^{\{e\}}$ (IV.33a) and $\tilde{\mathbb{M}}_{\text{I}}^{\{e\}} c^2$ (IV.40) are based upon the spherically symmetric approximation $[^p]A_0(r)$ for the potential $\{^p\}A_0(r, \vartheta)$ and also upon the same trial amplitude $\tilde{\Phi}(r)$ (III.50) with $\nu = 0$, so that the spherically symmetric Poisson constraint is satisfied in first order (i. e. $E_{\text{I}}^{\{e\}} - \tilde{\mathbb{M}}_{\text{I}}^{\{e\}} c^2 = 0$). But the consequence of this peculiarity is now that the non-relativistic constraint term $\tilde{\mathbb{N}}_{\text{G}}^{\{e\}}$ (IV.38) is built up exclusively by the anisotropic corrections:

$$\begin{aligned} \tilde{\mathbb{N}}_{\text{G}}^{\{e\}} &= (E_{\text{I}}^{\{e\}} + E_{\text{II}}^{\{e\}} + E_{\text{III}}^{\{e\}}) - (\tilde{\mathbb{M}}_{\text{I}}^{\{e\}} c^2 + \tilde{\mathbb{M}}_{\text{III}}^{\{e\}} c^2) \\ &= E_{\text{II}}^{\{e\}} + E_{\text{III}}^{\{e\}} - \tilde{\mathbb{M}}_{\text{III}}^{\{e\}} c^2 = - \frac{11}{120} \hbar c \alpha_s \beta . \end{aligned} \quad (\text{IV.42})$$

Collecting now all the partial results, i. e. the kinetic energy E_{kin} (IV.31) plus the gauge field energy (IV.33a)-(IV.33c) plus the Poisson constraint term (IV.42), and then substituting this back into the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (IV.29) yields the value of this functional on the chosen trial configuration $\{\tilde{\Phi}(r), \{^p\}A_0(r, \vartheta)\}$ in form of an energy function ($\tilde{\mathbb{E}}_{\Phi}(\beta)$, say) which is found to be of the following shape:

$$\tilde{\mathbb{E}}_{\Phi}(\beta) = \frac{e^2}{a_B} \left\{ (\beta a_B)^2 - \frac{481}{480} (\beta a_B) \right\} . \quad (\text{IV.43})$$

(Observe here also the value (III.49b) for the Lagrangean parameter $\lambda_{\text{G}}^{(e)}$). It is now this result (IV.43) which is well-suited for a first estimate of the influence of anisotropy. Namely, the *spherically symmetric approximation* does also produce an energy function

(i. e. $\mathbb{E}^{[IV]}(\beta, \nu)$, cf. (A.22)), which for the special case $\nu = 0$ looks as follows:

$$\mathbb{E}^{[IV]}(\beta, 0) = \frac{e^2}{a_B} \left\{ (2\beta a_B)^2 \cdot \varepsilon_{\text{kin}}(0) - (2\beta a_B) \cdot \varepsilon_{\text{pot}}(0) \right\} = \frac{e^2}{a_B} \left\{ (\beta a_B)^2 - (\beta a_B) \right\} \quad (\text{IV.44})$$

where the special values of the functions $\varepsilon_{\text{kin}}(\nu)$ and $\varepsilon_{\text{pot}}(\nu)$ may immediately be read off from the equations (A.27) ($\Rightarrow \varepsilon_{\text{kin}}(0) = \frac{1}{4}$) and from (IV.36) ($\Rightarrow \varepsilon_{\text{pot}}(0) = \frac{1}{2}$). Comparing now the anisotropic result (IV.43) to its present isotropic counterpart (IV.44) demonstrates clearly that the anisotropic corrections for the groundstate will amount to roughly 4 parts in 10^3 ! More concretely, one determines the groundstate energy as the minimal value of these energy functions (IV.43) and (IV.44) and thus finds for the “*anisotropic groundstate*” (IV.43)

$$\mathbb{E}_T^{\{1\}} \doteq \tilde{\mathbb{E}}_\Phi(\beta) \Big|_{\min} = -\frac{e^2}{4a_B} \cdot \left(\frac{481}{480} \right)^2 \simeq -\frac{e^2}{4a_B} \cdot 1.00417... \quad (\text{IV.45})$$

and for the “*isotropic groundstate*” (IV.44)

$$\begin{aligned} \mathbb{E}^{[IV]}(\beta, 0) \Big|_{\min} &= -\frac{e^2}{4a_B} \equiv E_{\text{conv}}^{(1)} \\ \left(\frac{e^2}{4a_B} = 6.8029... \text{ eV} \right). \end{aligned} \quad (\text{IV.46})$$

From these results it is now obvious that the influence of the anisotropy on the groundstate energy amounts to only 0.4%. It is true, our trial amplitude $\tilde{\Phi}(r)$ (IV.22a)-(IV.22b) with the fixation $\nu = 0$ is not the optimal choice for the groundstate; if one admits non-zero ν and carries through the *isotropic* (!) minimalization procedure, one will find the minimal value of the corresponding energy function at $-7.23... \text{ [eV]}$ for $\nu = -0.2049...$ (see **table 1** on p. 44 and fig.s 4a-4b of ref. [11]). This *anisotropic* lowering (IV.45) of the groundstate energy below that simple isotropic RST prediction (IV.46) (which despite its naïve deduction equals *exactly* the conventional prediction $E_{\text{conv}}^{(1)}$ (I.4)) must now be tested for the whole positronium spectrum. But since the excited states require here the use of (at least) a two-parameter trial amplitude, we have to admit the more realistic trial amplitudes $\tilde{\Phi}(r)$ (III.50) with $\nu \neq 0$ in connection with an *improved* (!) expansion

with respect to the magnitude of anisotropy (see **Sect. V**). Namely, the point here is that the present anisotropic groundstate lowering (IV.45) is actually false, as pleasant as its smallmess ($\sim 0,4\%$) may appear in the light of a perturbation expansion. Indeed, we will readily demonstrate now that an improved *expansion with respect to the magnitude of anisotropy*, not so naïve as the above proposal (IV.9), will for the excited states yield anisotropic corrections in the range of some 6% as opposed to the present 0,4% due to our naïve expansion (IV.9).

V Anisotropic Corrections for the Excited States

Since, for the treatment of the excited states (**App.C**), the expansion (IV.8)-(IV.9) of the anisotropic gauge potential $\{^p\}A_0(r, \vartheta)$ (IV.5) in combination with the lowest-order postulate (IV.25) has been revealed as being too naïve, we have to develop now a more systematic way of expanding the gauge potential around that spherically symmetric approximation $[^p]A_0(r)$ (IV.23). The crucial point here aims just at the very concept of the spherically symmetric approximation, being termed as $[^p]A_0(r)$. Naturally, one would associate to this approximation $[^p]A_0(r)$ the property that it represents the average of the original potential $\{^p\}A_0(r, \vartheta)$ on the 2-sphere, see equation (V.8) below; or rephrased in other words: the average of the anisotropic constituent ($\{^p\}A_{an}(r, \vartheta)$) of $\{^p\}A_0(r, \vartheta)$ on the 2-sphere must vanish, see equation (V.7) below. But these requirements are not satisfied by our naïve expansion (IV.8)-(IV.11e). Subsequently, we will iron out this preliminary deficiency of our anisotropy expansion and thus will obtain distinctly improved predictions for the positronium spectrum (cf. **table 2** below, p. 77, to the former **table 1**, p. 44).

1. Expansion around Spherically Symmetric Approximation

To this end, we recall the integral representation (III.37) of the spherically symmetric approximation $[^p]A_0(r)$ (for general ν) and use this for the desired expansion of $\{^p\}A_0(r, \vartheta)$ around $[^p]A_0(r)$, namely by putting

$$\begin{aligned}\{^p\}A_0(r, \vartheta) &= [^p]A_0(r) + (\{^p\}A_0(r, \vartheta) - [^p]A_0(r)) \\ &= \frac{\alpha_s}{8} \int \frac{d^3\vec{r}'}{r'} \frac{\tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|} + \frac{\alpha_s}{4\pi} \int \frac{d^3\vec{r}'}{r'} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) \frac{\tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|}.\end{aligned}\quad (\text{V.1})$$

Here, the second part is obviously to be considered as the truly anisotropic constituent $\{^p\}A^{an}(r, \vartheta)$, i. e. we define

$$\begin{aligned}\{^p\}A^{an}(r, \vartheta) &\doteq \{^p\}A_0(r, \vartheta) - [^p]A_0(r) \\ &= \frac{\alpha_s}{4\pi} \int \frac{d^3\vec{r}'}{r'} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) \frac{\tilde{\Phi}^2(r')}{\|\vec{r} - \vec{r}'\|}.\end{aligned}\quad (\text{V.2})$$

This anisotropic constituent of the gauge potential may now be expanded by use of equation (IV.8) which yields a series expansion quite similarly as shown by equation (IV.9)

$$\begin{aligned} \{p\}A^{\text{an}}(r, \vartheta) &= \{p\}A^I(\vartheta) \cdot \{p\}A^I(r) + \{p\}A^{II}(\vartheta) \cdot \{p\}A^{II}(r) + \{p\}A^{III}(\vartheta) \cdot \{p\}A^{III}(r) \\ &\quad + \{p\}A^{IV}(\vartheta) \cdot \{p\}A^{IV}(r) + \{p\}A^{V}(\vartheta) \cdot \{p\}A^{V}(r) + \dots \end{aligned} \quad (\text{V.3})$$

Although this looks very similar to the former expansion (IV.9), the individual terms are somewhat different especially concerning the angular pre-factors:

$$\{p\}A^I(\vartheta) \doteqdot \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) = 0 \quad (\text{V.4a})$$

$$\{p\}A^{II}(\vartheta) \doteqdot \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) (\hat{\vec{r}} \cdot \hat{\vec{r}}') = 0 \quad (\text{V.4b})$$

$$\{p\}A^{III}(\vartheta) \doteqdot \frac{3}{2} \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) (\hat{\vec{r}} \cdot \hat{\vec{r}}')^2 = \frac{3\pi}{16} (\cos^2 \vartheta - \frac{1}{3}) \quad (\text{V.4c})$$

$$\{p\}A^{IV}(\vartheta) \doteqdot \frac{5}{2} \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) (\hat{\vec{r}} \cdot \hat{\vec{r}}')^3 = 0 \quad (\text{V.4d})$$

$$\begin{aligned} \{p\}A^V(\vartheta) \doteqdot \frac{35}{8} \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) (\hat{\vec{r}} \cdot \hat{\vec{r}}')^4 &= \frac{105}{128} \pi \{ \cos^4 \vartheta + \cos^2 \vartheta \sin^2 \vartheta + \frac{3}{8} \sin^4 \vartheta - \frac{8}{15} \} \\ & \end{aligned} \quad (\text{V.4e})$$

⋮

These angular factors $\{p\}A^N(\vartheta)$ ($N = I, II, III, IV, V, \dots$) have zero average over the 2-sphere, i. e.

$$\int \frac{d\Omega}{4\pi} \{p\}A^N(\vartheta) = \frac{1}{4\pi} \int d\phi d\vartheta \sin \vartheta \{p\}A^N(\vartheta) = 0 , \quad (\text{V.5})$$

because of the commutativity of both angular integrations, i. e.

$$\begin{aligned} \int \frac{d\Omega}{4\pi} \{p\}A^N(\vartheta) &\simeq \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) \int \frac{d\Omega}{4\pi} (\hat{\vec{r}} \cdot \hat{\vec{r}}')^{N-1} \\ &= \int \frac{d\Omega'}{4\pi} \left(\frac{1}{\sin \vartheta'} - \frac{\pi}{2} \right) \cdot \frac{1}{N} = 0 . \end{aligned} \quad (\text{V.6})$$

Therefore the average of the anisotropic potential $\{p\}A^{\text{an}}(r, \vartheta)$ (V.3) is zero:

$$\int \frac{d\Omega}{4\pi} \{p\}A^{\text{an}}(r, \vartheta) \equiv 0 ; \quad (\text{V.7})$$

and thus the spherically symmetric approximation ${}^{[p]}A_0(r)$ (III.37), as the leading term of the series expansion (V.1)-(V.3), is revealed as the angular average of the general anisotropic potential $\{^p\}A_0(r, \vartheta)$ (IV.7), i. e.

$${}^{[p]}A_0(r) \equiv \int \frac{d\Omega}{4\pi} \{^p\}A_0(r, \vartheta) . \quad (\text{V.8})$$

Concerning the radial factors of the series expansion (V.3), one observes on account of the vanishing of the first two angular factors $\{^p\}A^I(\vartheta)$ (V.4a) and $\{^p\}A^{II}(\vartheta)$ (V.4b) that the first active non-trivial potential is that of third order

$$\{^p\}A^{III}(r) = \alpha_s \int dr' r' \frac{(rr')^2 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{5}{2}}} \equiv \{^p\}A_{III}(r) , \quad (\text{V.9})$$

cf. (IV.11c), and the next non-trivial one to be considered here is of fifth order (cf. (V.4d)-(V.4e))

$$\{^p\}A^V(r) = \alpha_s \int dr' r' \frac{(rr')^4 \cdot \tilde{\Phi}^2(r')}{(r^2 + r'^2)^{\frac{9}{2}}} \equiv \{^p\}A_V(r) , \quad (\text{V.10})$$

cf. (IV.11e). Thus the present expansion (V.1)-(V.3) of the gauge potential is essentially the same as the naïve one (IV.9), and differs from that former one only in the angular parts. Consequently, the hierarchical arrangement of magnitudes, as expressed in **Fig.IV.A**, should *in principle* apply also to the present expansion (V.1)-(V.3).

2. Energy Content of the Anisotropic Configurations

The present expansion around the spherically symmetric approximation has also some useful consequences with respect to the anisotropic energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (IV.29). The crucial point here is the circumstance that with the specification of the angular pre-factors $\{^p\}A^I(\vartheta)$, $\{^p\}A^{II}(\vartheta)$, ... one can integrate over these angular functions so that the *principle of minimal energy* becomes reduced to a purely radial problem for the remaining spherically symmetric fields ${}^{[p]}A_0(r)$, $\{^p\}A^{III}(r)$, $\tilde{\Phi}(r)$. This reduction to a spherically symmetric problem is carried through as follows:

The first consequence of the representation of the anisotropic potential $\{^{\text{p}}\}A_0(r, \vartheta)$ as a sum of two terms, cf. (V.1)

$$\{^{\text{p}}\}A_0(r, \vartheta) = [^{\text{p}}]A_0(r) + \{^{\text{p}}\}A^{\text{an}}(r, \vartheta), \quad (\text{V.11})$$

refers to its energy content $E_{\text{R}}^{(\text{e})}$ (II.36)

$$E_{\text{R}}^{(\text{e})} \Rightarrow E_{\text{R}}^{\{\text{e}\}} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3\vec{r} \|\vec{\nabla} \{^{\text{p}}\}A_0(r, \vartheta)\|^2 \quad (\text{V.12})$$

which appears now as a sum of three terms

$$E_{\text{R}}^{\{\text{e}\}} = E_{\text{R}}^{[\text{e}]} + E_{\text{an}}^{\{\text{e}\}} + E_{\text{mx}}^{\{\text{e}\}}. \quad (\text{V.13})$$

Here, the first term is the energy content of the spherically symmetric approximation $[^{\text{p}}]A_0(r)$

$$\begin{aligned} E_{\text{R}}^{[\text{e}]} &= -\frac{\hbar c}{4\pi\alpha_s} \int d^3\vec{r} \|\vec{\nabla} [^{\text{p}}]A_0(r)\|^2 \\ &= -\frac{\hbar c}{\alpha_s} \int_0^\infty dr \left(r \cdot \frac{d [^{\text{p}}]A_0(r)}{dr} \right)^2 \end{aligned} \quad (\text{V.14})$$

and is for our trial amplitude $\tilde{\Phi}(r)$ (III.50) explicitly given by

$$E_{\text{R}}^{[\text{e}]} = -\frac{e^2}{a_B} (2a_B \beta) \cdot \varepsilon_{\text{pot}}(\nu) \quad (\text{V.15})$$

where the potential function $\varepsilon_{\text{pot}}(\nu)$ is specified by equation (A.28) of **App. A**, see here also equation (A.22) and **App. D** of ref. [12]. Analogously, the second energy contribution $E_{\text{an}}^{\{\text{e}\}}$ is the energy content of the anisotropic part $\{^{\text{p}}\}A^{\text{an}}(r, \vartheta)$ of the gauge potential and is given by

$$E_{\text{an}}^{\{\text{e}\}} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3\vec{r} \|\vec{\nabla} \{^{\text{p}}\}A^{\text{an}}(r, \vartheta)\|^2. \quad (\text{V.16})$$

This result says that the anisotropy energy is always negative and therefore must increase the binding energy!

And finally, there is a mixed contribution $E_{\text{mx}}^{\{e\}}$ which is built up cooperatively by both parts of the gauge potential

$$E_{\text{mx}}^{\{e\}} = -\frac{\hbar c}{2\pi\alpha_s} \int d^3\vec{r} \left(\vec{\nabla}^{[p]} A_0(r) \right) \cdot \left(\vec{\nabla}^{\{p\}} A^{\text{an}}(r, \vartheta) \right) . \quad (\text{V.17})$$

But the interesting point with this last contribution is now that it actually vanishes

$$E_{\text{mx}}^{\{e\}} = 0 . \quad (\text{V.18})$$

This can easily be verified by simply observing the fact that the spherically symmetric approximation ${}^{[p]}A_0(r)$ does not depend upon the polar angles ϑ and ϕ so that

$$\vec{\nabla}^{[p]} A_0(r) = \frac{d {}^{[p]}A_0(r)}{dr} \vec{e}_r , \quad (\text{V.19})$$

and consequently the mixed term depends exclusively on the derivatives in radial direction ($\sim \vec{e}_r$), i. e. we have by use of the anisotropy expansion (V.3)

$$\begin{aligned} E_{\text{mx}}^{\{e\}} &= -\frac{\hbar c}{2\pi\alpha_s} \int d^3\vec{r} \frac{d {}^{[p]}A_0(r)}{dr} \cdot \frac{\partial {}^{\{p\}}A^{\text{an}}(r, \vartheta)}{\partial r} \\ &= -\frac{\hbar c}{2\pi\alpha_s} \left\{ \int_0^\infty dr r^2 \frac{d {}^{[p]}A_0(r)}{dr} \cdot \frac{d {}^{\{p\}}A^I(r)}{dr} \int d\Omega {}^{\{p\}}A^I(\vartheta) \right. \\ &\quad + \int_0^\infty dr r^2 \frac{d {}^{[p]}A_0(r)}{dr} \cdot \frac{d {}^{\{p\}}A^{II}(r)}{dr} \int d\Omega {}^{\{p\}}A^{II}(\vartheta) \\ &\quad + \int_0^\infty dr r^2 \frac{d {}^{[p]}A_0(r)}{dr} \cdot \frac{d {}^{\{p\}}A^{III}(r)}{dr} \int d\Omega {}^{\{p\}}A^{III}(\vartheta) + \dots \\ &\quad \left. + \int_0^\infty dr r^2 \frac{d {}^{[p]}A_0(r)}{dr} \cdot \frac{d {}^{\{p\}}A^N(r)}{dr} \int d\Omega {}^{\{p\}}A^N(\vartheta) + \dots \right\} . \end{aligned} \quad (\text{V.20})$$

Thus the vanishing mean value (V.6) of the angular factors ${}^{\{p\}}A^N(\vartheta)$ just validates the claim (V.18), and consequently the gauge field energy $E_R^{\{e\}}$ becomes composed exclusively by the two quadratic terms (V.14) and (V.16)

$$E_R^{\{e\}} = E_R^{[e]} + E_{\text{an}}^{\{e\}} . \quad (\text{V.21})$$

The intended reduction of the original angular-dependent variational problem to a purely radial problem must here be carried through only for this gauge field contribution

$E_R^{\{e\}}$ (V.21) because the isotropic part $E_R^{[e]}$ is already defined as a purely radial integral, cf. (III.45); and for the anisotropic part $E_{an}^{\{e\}}$ (V.16) one integrates over the angular pre-factor $\{p\}A^{III}(\vartheta)$ (V.4c) so that a purely radial integral over $\{p\}A^{III}(r)$ is left over, see equation (V.30) below.

Clearly, if one could solve exactly the Poisson equation (IV.28) for the anisotropic potential $\{p\}A_0(r, \vartheta)$, then the Poisson constraint (IV.38) would not be a point of concern because it would disappear trivially from the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (IV.29). But since we will not find such an exact solution for the anisotropic gauge potential, we are forced to briefly inspect the Poisson constraint with reference to that splitting (V.11) of the gauge potential into an isotropic and anisotropic part. Indeed, this splitting induces a corresponding splitting of (the non-relativistic version of) the original mass equivalent $M^{(e)}c^2$ (II.37) into a spherically symmetric part $\tilde{\mathbb{M}}^{[e]}c^2$ and an anisotropic part $\tilde{\mathbb{M}}_{an}^{\{e\}}c^2$:

$$\begin{aligned}\tilde{\mathbb{M}}^{\{e\}}c^2 &\doteq -\hbar c \int d^3\vec{r} \, \{p\}A_0(r, \vartheta) \frac{\tilde{\Phi}^2(r)}{4\pi r \sin \vartheta} \\ &= \tilde{\mathbb{M}}^{[e]}c^2 + \tilde{\mathbb{M}}_{an}^{\{e\}}c^2,\end{aligned}\quad (\text{V.22})$$

with the isotropic part being given by equation (III.48) and analogously the anisotropic part by

$$\tilde{\mathbb{M}}_{an}^{\{e\}}c^2 = -\frac{\hbar c}{4\pi} \int \frac{d^3\vec{r}}{r \sin \vartheta} \, \{p\}A^{an}(r, \vartheta) \cdot \tilde{\Phi}^2(r). \quad (\text{V.23})$$

Concerning here the intended reduction to a purely radial problem, one integrates again over the angular part and is then left with a radial integral, see equation (V.31) below.

As a further consequence of the splitting (V.11), the Poisson constraint $\tilde{\mathbb{N}}_G^{\{e\}}$ (IV.38) must then also be split up into two terms

$$\tilde{\mathbb{N}}_G^{\{e\}} = \tilde{\mathbb{N}}_G^{[e]} + \tilde{\mathbb{N}}_{an}^{\{e\}}, \quad (\text{V.24})$$

with the isotropic part $\tilde{\mathbb{N}}_G^{[e]}$ being given by

$$\tilde{\mathbb{N}}_G^{[e]} = E_R^{[e]} - \tilde{\mathbb{M}}^{[e]}c^2 \quad (\text{V.25})$$

and similarly the anisotropic part $\tilde{N}_{\text{an}}^{\{e\}}$ by

$$\tilde{N}_{\text{an}}^{\{e\}} = E_{\text{an}}^{\{e\}} - \tilde{M}_{\text{an}}^{\{e\}} c^2 . \quad (\text{V.26})$$

Now the interesting point with this splitting (V.24) is the following: Since both isotropic parts $E_R^{\{e\}}$ (V.14) and $\tilde{M}^{\{e\}} c^2$ (III.48) are built up by the spherically symmetric approximation $[p]A_0(r)$ and this potential is an *exact* solution of the (albeit *approximate*) Poisson equation (III.36), the spherically symmetric part $\tilde{N}_G^{\{e\}}$ (V.25) of the general Poisson constraint $\tilde{N}_G^{\{e\}}$ (V.24) is zero

$$\tilde{N}_G^{\{e\}} = 0 ; \quad (\text{V.27})$$

and consequently the general Poisson constraint $\tilde{N}_G^{\{e\}}$ will consist exclusively of the properly anisotropic part $\tilde{N}_{\text{an}}^{\{e\}}$:

$$\tilde{N}_G^{\{e\}} \Rightarrow \tilde{N}_{\text{an}}^{\{e\}} , \quad (\text{V.28})$$

whose vanishing must be considered separately (see below). Actually, this is the generalized reformulation of the former result (IV.40) for the simplified groundstate.

Thus, summarizing all the precedent partial results, the anisotropic energy functional $\tilde{E}_{[\Phi]}$ (IV.29) can be recast to the following $SO(3)$ symmetric form (inclusive all constraints) which then neatly displays the separation into the spherically symmetric and the anisotropic gauge field degrees of freedom:

$$\tilde{E}_{[\Phi]} \Rightarrow \tilde{E}_{\{\Phi\}} = 2E_{\text{kin}} + [E_R^{\{e\}} + \lambda_G^{(e)} \cdot \tilde{N}_G^{\{e\}}] + \{E_{\text{an}}^{\{e\}} + \lambda_G^{(e)} \cdot \tilde{N}_{\text{an}}^{\{e\}}\} + 2\lambda_S \cdot \tilde{N}_\Phi . \quad (\text{V.29})$$

This result will readily become the point of departure for the approximate calculation of the “anisotropic” binding energy of the two-body system. But let us first remark here that the present functional $\tilde{E}_{\{\Phi\}}$ (V.29) is to be understood in the sense that all angular factors are already integrated over so that we are left with a variational problem for the spherically symmetric fields $\tilde{\Phi}(r)$, $[p]A_0(r)$, $\{p\}A^{\text{III}}(r)$, $\{p\}A^{\text{V}}(r)$, ... The Poisson constraint term $\tilde{N}_G^{\{e\}}$ is re-included here because this gives us the freedom to try (if we wish) also other configurations $\{\tilde{\Phi}(r), [p]A_0(r)\}$ which eventually do not obey the spherically symmetric

Poisson constraint (V.27). The same does hold also with respect to the “anisotropic” Poisson constraint $\tilde{N}_{\text{an}}^{\{e\}}$ (V.26).

Observe now that all contributions to the anisotropic energy $\tilde{E}_{\{\Phi\}}$ (V.29) are well-defined by our precedent assumptions:

- (i) the kinetic energy E_{kin} is given in terms of the spherically symmetric wave amplitude $\tilde{\Phi}(r)$ by equations (III.42)-(III.44)
- (ii) the “spherically symmetric” gauge field energy $E_{\text{R}}^{[e]}$ reads in terms of the $SO(3)$ symmetric part ${}^{[p]}A_0(r)$ of the gauge potential as shown by equation (V.14)
- (iii) the “spherically symmetric” mass equivalent $\tilde{M}^{[e]}c^2$ is displayed by equation (III.48)
- (iv) the “anisotropic” gauge field energy $E_{\text{an}}^{\{e\}}$ (V.16) becomes by the restriction to its lowest-order contribution ${}^{[p]}A^{\text{III}}(r)$, cf. (V.3)

$$E_{\text{an}}^{\{e\}} = -\frac{\pi^2}{320} \frac{\hbar c}{\alpha_s} \int_0^\infty dr r^2 \left\{ \left(\frac{d {}^{[p]}A^{\text{III}}(r)}{dr} \right)^2 + 6 \left(\frac{{}^{[p]}A^{\text{III}}(r)}{r} \right)^2 \right\} \quad (\text{V.30})$$

- (v) the “anisotropic” mass equivalent $\tilde{M}_{\text{an}}^{\{e\}}c^2$ (V.23) is found to be of the following form

$$\tilde{M}_{\text{an}}^{\{e\}}c^2 = -\frac{\pi^2}{64} \hbar c \int_0^\infty dr r \tilde{\Phi}^2(r) \cdot {}^{[p]}A^{\text{III}}(r) \quad (\text{V.31})$$

where we are satisfied again with the first anisotropic correction ${}^{[p]}A^{\text{III}}(r)$.

3. Principle of Minimal Energy

With the (*anisotropic!*) trial configuration being specified now through the three *spherically symmetric (!)* fields $\tilde{\Phi}(r)$, ${}^{[p]}A_0(r)$, ${}^{[p]}A^{\text{III}}(r)$ one can look for the extremal equations due to the functional $\tilde{E}_{\{\Phi\}}$ (V.29) with respect to just these three fields. This may be done by prescribing the functional form of the three fields and equipping this form

with certain variational parameters $\{\beta, \nu_k\}$ and then determining the extremal points of the corresponding energy function over the parameter space (see the former equations (III.40)). An other method would consist in leaving the three fields unspecified for the time being and deducing for them a coupled system of differential equations from the *principle of minimal energy* (III.39). After having solved this system, one may substitute back the corresponding solutions into the energy functional $\tilde{E}_{\{\Phi\}}$ (V.29) in order to obtain its associated extremal value. An alternative “mixed” method would consist in prescribing the functional form (up to some variational parameters) of one or two of the three fields and determining the residual unprescribed field from its differential equation due to the *principle of minimal energy*.

In any case, it is very instructive to first deduce the system of extremal equations due to that functional $\tilde{E}_{\{\Phi\}}$ (V.29). The extremalization with respect to the spherically symmetric approximation ${}^{[p]}A_0(r)$ yields just again the former Poisson equation (III.36). Therefore the former link (III.37) of the spherically symmetric approximation ${}^{[p]}A_0(r)$ to the wave amplitude $\tilde{\Phi}(r)$ still persists which entails the continued validity of the Poisson constraint (V.27). But the converse is not true, i.e. the Schrödinger-like wave equation (III.34) receives an additional coupling to the anisotropic part ${}^{\{p\}}A^{\text{III}}(r)$ of the gauge potential ${}^{\{p\}}A_0(r, \vartheta)$ (V.3). Indeed, the extremalization of $\tilde{E}_{\{\Phi\}}$ (V.29) with respect to the wave amplitude $\tilde{\Phi}(r)$ generates the following modification of the original equation (III.34):

$$-\frac{\hbar^2}{2M} \left(\frac{d^2\tilde{\Phi}(r)}{dr} + \frac{1}{r} \frac{d\tilde{\Phi}(r)}{dr} \right) + \frac{\hbar^2}{2M} \frac{l_\varphi^2}{r^2} \tilde{\Phi}(r) - \hbar c \left[{}^{[p]}A_0(r) + \frac{\pi}{32} {}^{\{p\}}A^{\text{III}}(r) \right] \tilde{\Phi}(r) = E_* \cdot \tilde{\Phi}(r). \quad (\text{V.32})$$

Thus it becomes evident that the gauge field influences the *spherically symmetric* amplitude $\tilde{\Phi}(r)$ not only via its average potential ${}^{[p]}A_0(r)$, i.e. the spherically symmetric approximation (V.8), but also via its first anisotropy correction ${}^{\{p\}}A^{\text{III}}(r)$. However, this influence occurs in a very plausible way; namely the first anisotropy correction ${}^{\{p\}}A^{\text{III}}(r)$ is simply added to the spherically symmetric approximation ${}^{[p]}A_0(r)$ in order to build up a slightly modified (but still spherically symmetric) potential, to be considered as some

kind of effective potential! But observe also that the coupling of the amplitude $\tilde{\Phi}(r)$ to the first anisotropic correction $\{^p\}A^{III}(r)$ is (roughly) ten times ($\sim \frac{\pi}{32}$) weaker than its coupling to the average potential $[^p]A_0(r)$! On the other hand, it will readily turn out that the anisotropic correction $\{^p\}A^{III}(r)$ couples three times stronger to the amplitude $\tilde{\Phi}(r)$ than does the average potential $[^p]A_0(r)$, see equation (V.34) below. Therefore it is reasonable to take into account the anisotropy corrections for the gauge potential but not yet for the wave amplitude.

Finally, the extremal equation of $\tilde{\mathbb{E}}_{\{\Phi\}}$ (V.29) with respect to the anisotropic correction $\{^p\}A^{III}(r)$ must be determined. Since the latter field is contained only in two terms of $\tilde{\mathbb{E}}_{\{\Phi\}}$, namely the “anisotropic” energy $E_{\text{an}}^{\{e\}}$ (V.30) and the “anisotropic” mass equivalent $\tilde{\mathbb{M}}_{\text{an}}^{\{e\}}c^2$ (V.31), the variational process (δ_{III} , say) with respect to $\{^p\}A^{III}(r)$ becomes very simple

$$\delta_{III}\tilde{\mathbb{E}}_{\{\Phi\}} \stackrel{!}{=} 0 \Rightarrow \delta_{III}\left(E_{\text{an}}^{\{e\}} + \lambda_G^{(e)} \cdot \tilde{\mathbb{N}}_{\text{an}}^{\{e\}}\right) \stackrel{!}{=} 0 , \quad (\text{V.33})$$

with the “anisotropic” energy $E_{\text{an}}^{\{e\}}$ given by equation (V.30) and the mass equivalent $\tilde{\mathbb{M}}_{\text{an}}^{\{e\}}c^2$ by (V.31). The result of this extremalization process is the following Poisson-like equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{6}{r^2}\right) \{^p\}A^{III}(r) = -5\alpha_s \frac{\tilde{\Phi}^2(r)}{r} . \quad (\text{V.34})$$

Evidently, this equation owns some properties which are worthwhile to be mentioned briefly. Firstly, the coupling of the anisotropy potential $\{^p\}A^{III}(r)$ to the spherically symmetric wave amplitude $\tilde{\Phi}(r)$ is enhanced by a factor of $\frac{10}{\pi} \approx 3$, cf. the corresponding Poisson equation (III.36) for the spherically symmetric approximation (i.e. the average potential) $[^p]A_0(r)$. This hints at the circumstance that the deviation from the spherical symmetry is relatively large so that one (erroneously) tends to expect a correspondingly large amount of anisotropy energy $E_{\text{an}}^{\{e\}}$ (V.30) in comparison to the isotropic energy $E_R^{[e]}$ (V.14). Secondly, the last term ($\frac{\{^p\}A^{III}(r)}{r^2}$) on the left-hand side of equation (V.34) is necessary in order to ensure the former boundary conditions (IV.16) and (IV.19) for the anisotropy *corrections* of the gauge potential. Indeed, in the asymptotic region of three-

space ($r \rightarrow \infty$, $\tilde{\Phi}(r) \rightarrow 0$) the potential correction $\{^p\}A^{III}(r)$ has to obey the equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{6}{r^2} \right) \{^p\}A^{III}(r) \cong 0 \quad (\text{V.35})$$

which imposes upon the solution $\{^p\}A^{III}(r)$ the condition to vanish faster ($\sim \frac{1}{r^3}$) than the Coulomb potential ($\sim \frac{1}{r}$), i. e. more precisely (see **App. D**)

$$\{^p\}A^{III}(r) \cong \frac{2}{\pi} (2\nu + 3)(2\nu + 2) \cdot \frac{2\beta\alpha_s}{(2\beta r)^3} ; \quad (\text{V.36})$$

of course, this hints at the *quadrupole* character of this field (see **App. D**).

Finally, there is a further interesting point in connection with that “*quadrupole equation*” (V.34). This concerns the fact that the “anisotropic” Poisson constraint $\tilde{N}_{\text{an}}^{\{e\}}$ (V.26) vanishes whenever we can use an exact solution of the Poisson-like equation (V.34) as our trial potential $\{^p\}A^{III}(r)$, quite independently of the selection of a trial amplitude $\tilde{\Phi}(r)$ (see **App. D**). This is the same effect as does occur in connection with the “isotropic” Poisson constraint $\tilde{N}_G^{\{e\}}$ (V.25). Thus, provided that we are able to use exact solutions of both gauge field equations (III.36) and (V.34), then we can omit the corresponding constraint terms from the energy functional $\tilde{E}_{[\Phi]}$ (V.29). In this case, this functional becomes cut down to the following simple form:

$$\tilde{E}_{[\Phi]} \Rightarrow 2E_{\text{kin}} + E_R^{\{e\}} + E_{\text{an}}^{\{e\}} \equiv 2E_{\text{kin}} + E_R^{\{e\}} . \quad (\text{V.37})$$

Here it is also assumed that the selected trial amplitude is normalized to unity so that the normalization condition (III.46) is satisfied.

4. Energy Spectrum of the Excited States

After all these preparations, the calculation of the energy due to the excited states ($\nu > 0$) becomes now a simple matter: since the kinetic energy E_{kin} is proportional to the *square* of the variational parameter β , cf. (III.52)-(III.53); and since furthermore the total

gauge field energy $E_R^{\{e\}}$ (V.21) is a *linear* function of β (see equation (E.9a) of **App. E**), the extremalization process (III.40), or more concretely

$$\frac{\partial \mathbb{E}^{\{IV\}}(\beta, \nu)}{\partial \beta} = 0 \quad (\text{V.38a})$$

$$\frac{\partial \mathbb{E}^{\{IV\}}(\beta, \nu)}{\partial \nu} = 0 \quad (\text{V.38b})$$

with

$$\mathbb{E}^{\{IV\}}(\beta, \nu) = \frac{e^2}{a_B} \left\{ (2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (2a_B \beta) \cdot \varepsilon_{\text{tot}}^{\{e\}}(\nu) \right\}, \quad (\text{V.39})$$

yields again the desired energy values $\mathbb{E}_\phi^{\{n\}}$, namely as the minimal values of the reduced energy function $\mathbb{E}_{\{\nu\}}^\phi$

$$\mathbb{E}_\phi^{\{n\}} \doteq \mathbb{E}_{\{\nu\}}^\phi|_{\min}. \quad (\text{V.40})$$

Here, the reduced energy function $\mathbb{E}_{\{\nu\}}^\phi$ is again defined through

$$\mathbb{E}_{\{\nu\}}^\phi \doteq -\frac{e^2}{4a_B} \cdot S_\phi^{\{a\}}(\nu) \quad (\text{V.41})$$

with the “anisotropic” spectral function $S_\phi^{\{a\}}(\nu)$ being itself defined through

$$S_\phi^{\{a\}}(\nu) \doteq \frac{\varepsilon_{\text{tot}}^{\{e\}}(\nu)^2}{\varepsilon_{\text{kin}}(\nu)}. \quad (\text{V.42})$$

The (dimensionless) total potential function $\varepsilon_{\text{tot}}^{\{e\}}(\nu)$ is given by equation (E.9b) of **App. E** and is obviously nothing else than the “anisotropic” generalization of the former $\varepsilon_{\text{pot}}(\nu)$ (A.28). Thus the present energy function $\mathbb{E}^{\{IV\}}(\beta, \nu)$ (V.39) is the “anisotropic” generalization of the “isotropic” $\mathbb{E}^{\{IV\}}(\beta, \nu)$ (III.55) so that it merely remains to determine again the extremal values of the spectral function $S_\phi^{\{a\}}(\nu)$ (V.42) for any principal quantum number n_ϕ ($= l_\phi + 1$); for the numerical details see **App. F**.

The **table 2** (below) displays the RST predictions of the positronium energy $\mathbb{E}_\phi^{\{n\}}$ (V.40) in an arrangement quite similar to the results of the spherically symmetric approximation in **table 1** (p.44). Here it becomes obvious that the deviations from the conventional

results (last column in **tables 1** and **2**) are considerably reduced through the inclusion of the anisotropy corrections. Indeed, defining the “anisotropic” deviations by

$$\Delta_T(\nu_*^{\{n\}}) \doteq \frac{E_{\text{conv}}^{(n)} - \mathbb{E}_\varphi^{\{n\}}}{E_{\text{conv}}^{(n)}} \quad (\text{V.43})$$

(last column of **table 2**) in a quite analogous manner to their “isotropic” counterparts $\Delta_T(\nu_*^{[n]})$ (F.6) (last column of **table 1**), one clearly realizes that the “*anisotropic*” deviations (V.43) in **table 2** amount to less than half of the “*isotropic*” deviations (**table 1**). Observe here that the average $\overline{\Delta_{\{T\}}}$ of the deviations (V.43), being defined by

$$\overline{\Delta_{\{T\}}} \doteq \frac{1}{14} \sum_{n_\varphi} |\Delta_T(\nu_*^{\{n\}})| , \quad (\text{V.44})$$

does amount now to $\overline{\Delta_{\{T\}}} = 3,1\%$ in comparison to the corresponding former deviation $\overline{\Delta_{[T]}} = 7,7\%$ for the spherically symmetric approximation (**table 1**). The ground-state ($n_\varphi = 1$) is disregarded here because the presently applied *electrostatic approximation* is supposed to fail for the lowest energy eigenstate (see the discussion of this in the precedent paper [11]).

Clearly such a result suggests to consider the higher-order approximations which eventually do shift the RST predictions even closer to their conventional counterparts, see **Fig.V.A** below.

n_ϕ $= (l_\phi + 1)$	ν_n	$S_n^{\{a\}}(\nu = \nu_n)$ (V.41)	$S_n _{\max}$ App.F	$\mathbb{E}_\phi^{\{n\}}$ [eV] (V.40)	$E_{\text{conv}}^{(n)}$ [eV] (I.4)	$\Delta_T(\nu_*^{\{n\}})$ (V.43)
2	2	2.42009e-01	2.42186e-01	-1.647e+00	-1.701e+00	3.1
3	4	1.05465e-01	1.05479e-01	-7.175e-01	-7.558e-01	5.1
4	6	5.92349e-02	5.92388e-02	-4.030e-01	-4.251e-01	5.2
5	17/2	3.80558e-02	3.80558e-02	-2.589e-01	-2.721e-01	4.9
6	11	2.65700e-02	2.65701e-02	-1.807e-01	-1.890e-01	4.3
10	45/2	9.77183e-03	9.77187e-03	-6.647e-02	-6.802e-02	2.3
15	77/2	4.42916e-03	4.42916e-03	-3.013e-02	-3.023e-02	0.3
20	113/2	2.52621e-03	2.52621e-03	-1.718e-02	-1.701e-02	-1.0
25	76	1.63360e-03	1.63360e-03	-1.111e-02	-1.088e-02	-2.1
30	193/2	1.14365e-03	1.14365e-03	-7.779e-03	-7.558e-03	-2.9
35	118	8.45729e-04	8.45729e-04	-5.753e-03	-5.553e-03	-3.6
40	141	6.51019e-04	6.51019e-04	-4.428e-03	-4.251e-03	-4.2
50	189	4.20206e-04	4.20206e-04	-2.858e-03	-2.721e-03	-5.0

Table 2: *RST predictions $\mathbb{E}_\phi^{\{n\}}$ (V.40) including the Anisotropic Corrections*

The “anisotropic” RST predictions $\mathbb{E}_\phi^{\{n\}}$ (V.40) deviate only half as much from the conventional predictions $E_{\text{conv}}^{(n)}$ as is the case for the spherically symmetric approximation of lowest order (**table 1**). Indeed, the average deviation $\overline{\Delta_{\{T\}}}$ (V.44) is now $\overline{\Delta_{\{T\}}} = 3, 1\%$ in place of $\overline{\Delta_{[T]}} = 7, 7\%$ for the spherically symmetric approximation. Observe also that for quantum number $n_\phi \approx 15$ the deviation is minimal as predicted by an inspection of the “isotropic” and “anisotropic” deviations $\Delta_{\{\nu\}}$ and $\Delta_T(\nu_*^{[n]})$ in **Fig.F.II**, **App.F**

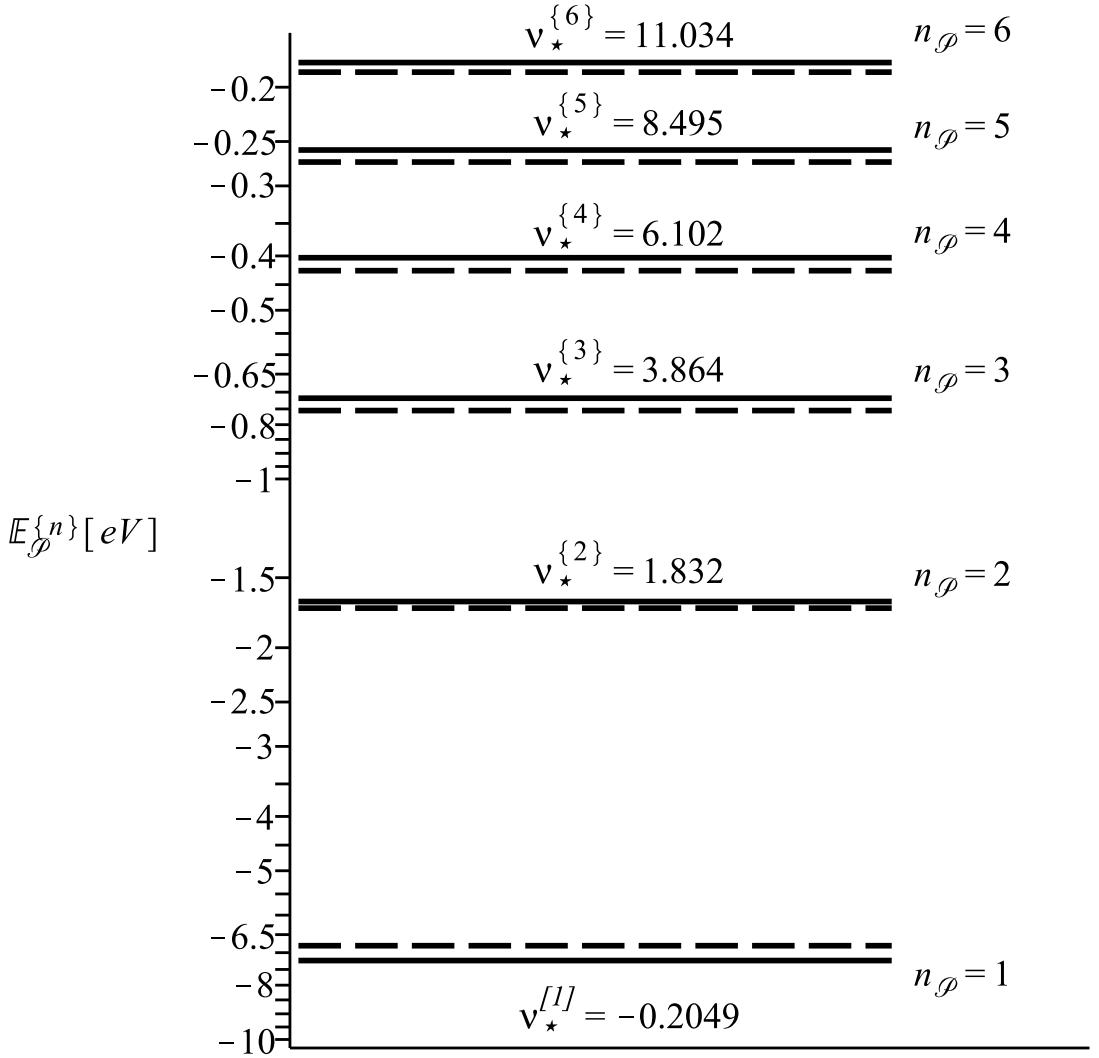


Fig. V.A *Energy Spectrum $\mathbb{E}_\phi^{\{n\}}$ (V.40) inclusive Anisotropy Corrections*

The inclusion of the anisotropy corrections diminishes the deviations of the RST predictions from their conventional counterparts by (roughly) 50%, cf. **Fig.III.A**: This improvement suggests that the regard of the anisotropy effects of higher approximation order will shift the RST predictions (solid lines) even closer towards their conventional counterparts (broken lines).

VI Improving the Spherically Symmetric Approximation

Concerning the essential point with the anisotropy corrections, it is instructive to first recall those results being collected in **table 2** on p. 77. These results let appear the magnitude of the anisotropy corrections in the range from 3% (for the first excited state, $n_\phi = 2$) up to 0.3% (for the excited state with principal quantum number $n_\phi = 15$). Evidently, the consideration of the anisotropy corrections in **Sect. V** improves the “isotropic” RST predictions (**table 1**) by (roughly) 50%. Surely, the higher-order corrections of the *anisotropic* type can be expected to shift the RST predictions further towards their conventional counterparts (I.4); but for the moment we are rather interested in testing the extent to which further improvements of the predictions may emerge *within the framework of the spherically symmetric approximation* itself (\rightsquigarrow isotropic corrections).

In this sense, we study now the following three-parameter generalization $\tilde{\Phi}_b(r)$ of the former two-parameter ansatz $\tilde{\Phi}(r)$ (III.50)-(III.51):

$$\tilde{\Phi}_b(r) = \Phi_* r^\nu (b_0 + b_1 r) e^{-\beta r} . \quad (\text{VI.1})$$

Here, the additional variational parameters are the (real) constants b_0, b_1 whose presence entails a certain generalization of the normalization constant Φ_* (III.51) so that the general normalization condition (III.38) becomes specified down to the following form

$$p_0^2 + 4(\nu + 1) \cdot p_0 p_1 + (2\nu + 3)(2\nu + 2) \cdot p_1^2 = 1 . \quad (\text{VI.2})$$

Here, the parameters p_0, p_1 are merely some convenient modification of the original ansatz parameters b_0, b_1 (VI.1), i.e.

$$p_0 \doteq \sqrt{\frac{\pi}{2} \cdot \Gamma(2\nu + 2)} \frac{\Phi_*}{(2\beta)^{\nu+1}} \cdot b_0 \quad (\text{VI.3a})$$

$$p_1 \doteq \sqrt{\frac{\pi}{2} \cdot \Gamma(2\nu + 2)} \frac{\Phi_*}{(2\beta)^{\nu+2}} \cdot b_1 . \quad (\text{VI.3b})$$

Clearly, for $p_1 \rightarrow 0, p_0 \rightarrow 1$ one is led back to the former two-parameter ansatz (III.50)-(III.51). Observe also that the present normalization condition (VI.2) is a slight generalization of the former condition (IV.41) of ref. [14] which emerges from the present condition (VI.2) through putting ν to zero ($\nu \rightarrow 0$).

1. Improved Energy Function

This new trial amplitude $\tilde{\Phi}_b(r)$ (VI.1) must now be used in order to calculate anew the kinetic energy E_{kin} (III.42)-(III.44) and the gauge field energy $E_R^{[e]}$ (III.45) with its corresponding mass equivalent $\tilde{M}^{[e]}c^2$ (III.48). Both objects will then obey the Poisson identity (III.47) provided the electrostatic potential $[p]A_0(r)$ is taken again as the exact solution of the spherically symmetric Poisson equation (III.36). Thus, both constraints (III.46) and (III.47) will be automatically satisfied and therefore the non-relativistic energy functional $\tilde{E}_{[\Phi]}$ (III.41) will consist exclusively of its physical contributions (i. e. kinetic energy and gauge field energy):

$$\tilde{E}_{[\Phi]} \Rightarrow \tilde{E}_{[\Phi]}^{\text{IV}} \doteq 2E_{\text{kin}} + E_R^{[e]} . \quad (\text{VI.4})$$

Clearly, this is again the non-relativistic version of the former relativistic case $E_{[\text{T}]}^{\text{(IV)}}$ (II.33).

Turning here first to the kinetic energy E_{kin} , one recalls that this energy contribution is the sum of the radial part ${}^{(r)}E_{\text{kin}}$ and the longitudinal part ${}^{(\theta)}E_{\text{kin}}$, cf. equation (III.42). Both parts must now be calculated by use of the generalized trial amplitude $\tilde{\Phi}_b(r)$ (VI.1). This yields first for the radial part ${}^{(r)}E_{\text{kin}}$ the usual form:

$${}^{(r)}E_{\text{kin}} = \frac{e^2}{2a_B} (2\beta a_B)^2 \cdot {}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) . \quad (\text{VI.5})$$

Here, the kinetic function of the radial type ${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ is defined in terms of the dimensionless form $\tilde{\Phi}_{\nu p}(y)$ of the original trial amplitude $\tilde{\Phi}_b(r)$ (VI.1) through

$$\begin{aligned} {}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) &= \frac{1}{\Gamma(2\nu+2)} \int dy y \left[\frac{d}{dy} \tilde{\Phi}_{\nu p}(y) \right]^2 \\ &\quad (\tilde{\Phi}_{\nu p}(y) \doteq y^\nu (p_0 + p_1 y) e^{-\frac{y}{2}}, \text{ see App. G}) . \end{aligned} \quad (\text{VI.6})$$

The explicit calculation lets emerge this radial kinetic function in the following shape

$${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) = \frac{p_0^2}{4(2\nu + 1)} + \frac{\nu}{2\nu + 1} \cdot p_0 p_1 + \frac{\nu + 1}{2} \cdot p_1^2, \quad (\text{VI.7})$$

i.e. a quadratic polynomial with respect to the variational parameters p_0, p_1 . Clearly, when the parameter p_1 tends to zero ($p_1 \rightarrow 0$) the present radial function ${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.7) collapses to the corresponding *radial part* of the result (III.53) which is due to the former two-parameter trial amplitude $\tilde{\Phi}(r)$ (III.50).

A similar line of arguments may also be applied to the *longitudinal* kinetic energy ${}^{(\vartheta)}E_{\text{kin}}$ (III.44) which then adopts an analogous form

$${}^{(\vartheta)}E_{\text{kin}} = \frac{e^2}{2a_B} (2\beta a_B)^2 l_\varphi^2 \cdot {}^{(\vartheta)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) \quad (\text{VI.8})$$

with the longitudinal type of kinetic energy function ${}^{(\vartheta)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ being found as

$${}^{(\vartheta)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) = \frac{p_0^2}{2\nu(2\nu + 1)} + \frac{2p_0 p_1}{2\nu + 1} + p_1^2. \quad (\text{VI.9})$$

Clearly, this quadratic form is again the longitudinal counterpart of the radial object ${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.7); and if the variational parameter p_1 tends to zero ($\rightsquigarrow p_0 \rightarrow 1$) one ends up here with the *longitudinal part* of the former $\varepsilon_{\text{kin}}(\nu)$ (III.53). Thus summarizing the result for the kinetic energy E_{kin} (III.42) as the sum of the radial and longitudinal parts, one ultimately arrives at

$$E_{\text{kin}} = \frac{e^2}{2a_B} (2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu, p_0, p_1) \quad (\text{VI.10})$$

with the total kinetic function $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ emerging here as the sum of the radial and longitudinal parts:

$$\begin{aligned} \varepsilon_{\text{kin}}(\nu, p_0, p_1) &\doteq {}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) + {}^{(\vartheta)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) \cdot l_\varphi^2 \\ &= \frac{\nu + 2l_\varphi^2}{4\nu(2\nu + 1)} \cdot p_0^2 + \frac{\nu + 2l_\varphi^2}{2\nu + 1} \cdot p_0 p_1 + \left(\frac{\nu + 1}{2} + l_\varphi^2 \right) \cdot p_1^2. \end{aligned} \quad (\text{VI.11})$$

As a consistency check one easily verifies that in the limit $p_1 \rightarrow 0$ this three-parameter result (VI.11) collapses again to the former result $\varepsilon_{\text{kin}}(\nu)$ (III.53) for the two-parameter

variational ansatz. For $\nu = 0$ and $l_\varphi = 0$, the present kinetic energy E_{kin} (VI.10) agrees with the former kinetic energy E_{kin} (IV.22a)-(IV.22b) of ref. [14].

The gauge field energy $E_R^{[e]}$ as the second constituent of the energy functional $\mathbb{E}_{[\Phi]}^{(\text{IV})}$ (VI.4) is considerably more complicated than the kinetic energy E_{kin} . Here, the Poisson identity is of help in order to find the simplest form of this energy contribution (see **App.G** for the details). Summarizing the results, one finds the desired gauge field energy $E_R^{[e]}$ (III.45) to look as follows:

$$E_R^{[e]} = -\frac{e^2}{a_B} (2a_B \beta) \cdot \varepsilon_{\text{pot}}(\nu, p_0, p_1) . \quad (\text{VI.12})$$

Here, the *total potential function* $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ is obviously the generalization of the former potential function $\varepsilon_{\text{pot}}(\nu)$ (III.54) which for the simple trial amplitude $\tilde{\Phi}(r)$ (III.50) is explicitly given by equation (A.28) of **App. A**. But clearly, the present generalized trial amplitude $\tilde{\Phi}_b(r)$ (VI.1) must now entail a more complicated potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$; and indeed, the latter function is found to be of the following form:

$$\begin{aligned} \varepsilon_{\text{pot}}(\nu, p_0, p_1) = & p_0^4 \cdot \varepsilon_{\text{pot}}(\nu) + 4p_0^3 p_1 \cdot \varepsilon_I(\nu) + 4p_0^2 p_1^2 \cdot \varepsilon_{II}(\nu) + 4p_0 p_1^3 \cdot \varepsilon_{III}(\nu) \\ & + p_1^4 \cdot \varepsilon_{IV}(\nu) , \end{aligned} \quad (\text{VI.13})$$

cf. equation (G.16) of **App. G**.

This is obviously a fourth-order polynomial with respect to the variational parameters p_0, p_1 (VI.3a)-(VI.3b) where the four additional coefficients $\varepsilon_I, \dots, \varepsilon_{IV}$ are ordinary functions of the second variational parameter ν . Concerning their specific shape, one finds (see **App. G**) that there are certain interrelationships so that it is sufficient to specify in detail only three of them (e.g. $\varepsilon_{\text{pot}}, \varepsilon_I, \varepsilon_{II}$) and the remaining two (i.e. ε_{III} and ε_{IV}) are then related to the first three in a simple way. More concretely, the first *auxiliary potential function* $\varepsilon_I(\nu)$ is given quite generally in terms of the (dimensionless) potential $a_\nu(y)$ through

$$\begin{aligned} \varepsilon_I(\nu) &= -\frac{1}{\Gamma(2\nu+2)^2} \int_0^\infty dy y^{2\nu+2} e^{-y} \cdot a_\nu(y) \\ &\equiv -\frac{1}{\Gamma(2\nu+2)^2} \int_0^\infty dy y^{2\nu+1} e^{-y} \cdot a_{\nu+\frac{1}{2}}(y) . \end{aligned} \quad (\text{VI.14})$$

Here, the potential $a_\nu(y)$ is the solution of the Poisson-like equation

$$\frac{d^2 a_\nu(y)}{dy^2} + \frac{2}{y} \frac{da_\nu(y)}{dy} = y^{2\nu-1} \cdot e^{-y} \quad (\text{VI.15})$$

which essentially is a dimensionless form of the original Poisson equation (III.36). Therefore the solution can easily be specified as

$$a_\nu(y) = -\Gamma(2\nu+2) \cdot \left\{ 1 - e^{-y} \cdot \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu+2+n)} y^{2\nu+n} \right\}, \quad (\text{VI.16})$$

cf. equation (G.13a) of **App. G**; and if this is used in order to explicitly calculate the auxiliary function $\varepsilon_I(\nu)$ (VI.14) one ends up with

$$\begin{aligned} \varepsilon_I(\nu) &= \frac{2\nu+2}{2\nu+1} \cdot \left\{ 1 - \frac{1}{\Gamma(2\nu+3) \cdot 2^{4\nu+3}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+3+n)}{\Gamma(2\nu+2+n)} \right\} \\ &= 1 - \frac{1}{\Gamma(2\nu+2) \cdot 2^{4\nu+3}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+3+n)}{\Gamma(2\nu+3+n)}. \end{aligned} \quad (\text{VI.17})$$

Next, the second coefficient $\varepsilon_{II}(\nu)$ of $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ in (VI.13) turns out to be the sum of two contributions, i. e.

$$\varepsilon_{II}(\nu) = \varepsilon'_{II}(\nu) + \varepsilon''_{II}(\nu) \quad (\text{VI.18})$$

where the first part is related to the well-known $\varepsilon_{\text{pot}}(\nu)$ through

$$\varepsilon'_{II}(\nu) = (2\nu+2)^2 \cdot \varepsilon_{\text{pot}}|_{\nu+\frac{1}{2}} \quad (\text{VI.19})$$

and the second part is given by

$$\begin{aligned} \varepsilon''_{II}(\nu) &= \frac{(\nu+1)(2\nu+3)}{2\nu+1} \left\{ 1 - \frac{1}{\Gamma(2\nu+4) \cdot 2^{4\nu+4}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+4+n)}{\Gamma(2\nu+2+n)} \right\} \\ &= 2(\nu+1) \left\{ 1 - \frac{1}{\Gamma(2\nu+2) \cdot 2^{4\nu+4}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+4+n)}{\Gamma(2\nu+4+n)} \right\}. \end{aligned} \quad (\text{VI.20})$$

Finally, as mentioned above, the last two coefficients $\varepsilon_{III}(\nu)$ and $\varepsilon_{IV}(\nu)$ in (VI.13) may be expressed in terms of the precedent potential functions which are to be shifted as follows:

$$\varepsilon_{III}(\nu) = (2\nu+2)^2 \cdot \varepsilon_I|_{\nu+\frac{1}{2}} \quad (\text{VI.21a})$$

$$\varepsilon_{IV}(\nu) = (2\nu+3)^2 \cdot (2\nu+2)^2 \cdot \varepsilon_{\text{pot}}|_{\nu+1}. \quad (\text{VI.21b})$$

Thus the total potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ (VI.13) ultimately appears as a well-defined function of the variational parameters ν and p_0, p_1 ; and if this is substituted back into the gauge field energy $E_R^{[e]}$ (VI.12) we obtain this quantity, as desired, as a function of all four variational parameters $\{\beta; \nu, p_0, p_1\}$

$$E_R^{[e]} = -\frac{e^2}{a_B} (2a_B \beta) \cdot \{ p_0^4 \cdot \varepsilon_{\text{pot}}(\nu) + 4p_0^3 p_1 \cdot \varepsilon_I(\nu) + 4p_0^2 p_1^2 \cdot \varepsilon_{II}(\nu) + 4p_0 p_1^3 \cdot \varepsilon_{III}(\nu) + p_1^4 \cdot \varepsilon_{IV}(\nu) \} . \quad (\text{VI.22})$$

Here, one is easily convinced that for $p_1 \rightarrow 0$ this four-parameter energy of the gauge field actually collapses to the two-parameter result (III.54) being due to the simpler trial amplitude (III.50).

But now that both the kinetic energy E_{kin} and the gauge field energy $E_R^{[e]}$ are at hand in their improved versions, cf. (VI.10)-(VI.11) and (VI.22), one can add them together in order to find from the energy functional $\mathbb{E}_{[\Phi]}^{(IV)}$ (VI.4) the corresponding energy function $\mathbb{E}^{(IV)}(\beta; \nu, p_0, p_1)$ which then appears in the form

$$\mathbb{E}^{(IV)}(\beta; \nu, p_0, p_1) = \frac{e^2}{a_B} \{ (2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu, p_0, p_1) - (2a_B \beta) \cdot \varepsilon_{\text{pot}}(\nu, p_0, p_1) \} . \quad (\text{VI.23})$$

Of course, this is again the p -generalized form of the simple predecessor $\mathbb{E}^{(IV)}(\beta, \nu)$ (III.55).

2. Principle of Minimal Energy

With an improved energy function $\mathbb{E}^{(IV)}(\beta; \nu, p_0, p_1)$ being at hand now, one can next apply the principle of minimal energy (III.39)-(III.40) in order to look for the extremal points of that function. First, turn here to the determination of the first variational parameter β in terms of ν and p by exploiting the first of the equations (III.40). More concretely, the requirement

$$\frac{\partial \mathbb{E}^{(IV)}(\beta; \nu, p_0, p_1)}{\partial \beta} = 0 \quad (\text{VI.24})$$

yields the equilibrium value (β_*) of β as

$$2a_B \beta_* = \frac{1}{2} \cdot \frac{\varepsilon_{\text{pot}}(\nu, p_0, p_1)}{\varepsilon_{\text{kin}}(\nu, p_0, p_1)} , \quad (\text{VI.25})$$

and if this is substituted back into the original energy function $\mathbb{E}^{(\text{IV})}(\beta; \nu, p_0, p_1)$ (VI.23) one obtains the reduced energy function $\mathbb{E}_T(\nu, p_0, p_1)$ in the following form:

$$\mathbb{E}_T(\nu, p_0, p_1) \doteq \mathbb{E}^{(\text{IV})}(\beta; \nu, p_0, p_1) \Big|_{\beta=\beta_*} = -\frac{e^2}{4a_B} \cdot S_\phi(\nu, p_0, p_1) , \quad (\text{VI.26})$$

where the improved spectral function $S_\phi(\nu, p_0, p_1)$ is given now by

$$S_\phi(\nu, p_0, p_1) \doteq \frac{\varepsilon_{\text{pot}}^2(\nu, p_0, p_1)}{\varepsilon_{\text{kin}}(\nu, p_0, p_1)} . \quad (\text{VI.27})$$

Clearly, this is again the p -generalization of the simple spectral function (III.56b) which is due to the simpler trial ansatz (III.50). Indeed, for $p_1 \rightarrow 0$ the present three-parameter result $S_\phi(\nu, p_0, p_1)$ (VI.27) becomes reduced to its one-parameter predecessor $S_\phi(\nu)$ (III.56b).

3. Simplified Groundstate Demonstration

The improving effect due to the presence of the additional variational parameters p_0, p_1 may be roughly estimated by fixing the parameter ν in equation (VI.27) and thus discussing the spectral function $S_\phi(\nu, p_0, p_1)$ exclusively as a function of p_0, p_1 . If one knew the optimal value of ν , one could find in this way the desired extremal value of the energy function $\mathbb{E}_T(\nu, p_0, p_1)$ (VI.26). But for the moment we will be satisfied with only a moderate improvement of the results of **Sect. III** which are due to the simpler variational ansatz (III.50), i.e. we will base our improvement upon those values $\nu_*^{[n]}$ which are displayed in **table 1**. Recall that those results yielded a deviation of (roughly) 10% from the conventional predictions within the framework of the *two-parameter* amplitude $\tilde{\Phi}(r)$ (III.50).

For the sake of a transparent but sufficiently detailed demonstration of our improvement, we will restrict ourselves here to the groundstate situation ($n_\varphi = 1$) and, properly speaking, this would imply that we have to choose $\nu_* = -0.2049\dots$ (see **table 1**, first line). However, in order to keep our groundstate demonstration as uncomplicated as possible, we are satisfied with choosing $\nu = 0$. This choice reduces our four-parameter amplitude $\tilde{\Phi}_b(r)$ (VI.1) to a three-parameter trial ansatz which (for $p_1 = 0$) *incidentally* predicts *exactly* the same groundstate energy as the conventional theory (I.4), see the discussion of this in ref.s [11, 18]. It is true, a more realistic choice for the groundstate would be $\nu_* = -0.2049$ (see the first line of **table 1**), but this would render the intended demonstration unacceptably complicated, inasmuch the groundstate ($n_\varphi = 1 \Leftrightarrow l_\varphi = 0$) is in any case badly predicted by the present *electrostatic* approximation.

By these arrangements, the two-dimensional problem of looking for the extremal values of the energy function $\mathbb{E}_T(\nu, p_0, p_1)$ (VI.26)-(VI.27) becomes reduced to a one-dimensional problem, namely to look for the extremal values of the function $\mathbb{E}_T^{[0]}(p_0, p_1)$

$$\mathbb{E}_T^{[0]}(p_0, p_1) \doteq \mathbb{E}_T(\nu, p_0, p_1) \Big|_{\nu=0} . \quad (\text{VI.28})$$

Or equivalently, this means to look for the extremal values of the reduced spectral function $S_\varphi^{[0]}(p_0, p_1) \doteq S_\varphi(0, p_0, p_1)$

$$S_\varphi^{[0]}(p_0, p_1) \doteq \frac{\varepsilon_{\text{pot}}^2(0, p_0, p_1)}{\varepsilon_{\text{kin}}(0, p_0, p_1)} . \quad (\text{VI.29})$$

Here, the general kinetic function $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.11) becomes reduced to (observe $l_\varphi = 0$)

$$\varepsilon_{\text{kin}}(0, p_0, p_1) = \frac{1}{4}p_0^2 + \frac{1}{2}p_1^2 \doteq \tilde{\varepsilon}_{\text{kin}}(p_0, p_1) \quad (\text{VI.30})$$

and finally the reduced potential function $\tilde{\varepsilon}_{\text{pot}}(p_0, p_1) \doteq \varepsilon_{\text{pot}}(0, p_0, p_1)$ is deduced from $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ (VI.13) as follows

$$\tilde{\varepsilon}_{\text{pot}}(p_0, p_1) = p_0^4 \cdot \varepsilon_{\text{pot}}(0) + 4p_0^3 p_1 \cdot \varepsilon_I(0) + 4p_0^2 p_1^2 \cdot \varepsilon_{II}(0) + 4p_0 p_1^3 \cdot \varepsilon_{III}(0) + p_1^4 \cdot \varepsilon_{IV}(0) , \quad (\text{VI.31})$$

i. e. by reference to the table in **App.G**

$$\tilde{\varepsilon}_{\text{pot}}(p_0, p_1) = \frac{1}{2}p_0^4 + 3p_0^3 p_1 + \frac{17}{2}p_0^2 p_1^2 + \frac{25}{2}p_0 p_1^3 + \frac{33}{4}p_1^4 . \quad (\text{VI.32})$$

Thus the reduced spectral function $S_\phi^{[0]}(p)$ (VI.29) is ultimately found to be of the following form

$$S_\phi^{[0]}(p_0, p_1) = \frac{\tilde{\varepsilon}_{\text{pot}}(p_0, p_1)^2}{\tilde{\varepsilon}_{\text{kin}}(p_0, p_1)} = \frac{(p_0^4 + 6p_0^3p_1 + 17p_0^2p_1^2 + 25p_0p_1^3 + \frac{33}{2}p_1^4)^2}{p_0^2 + 2p_1^2} . \quad (\text{VI.33})$$

For determining the local extrema of this spectral function (VI.33), one has to observe the constraint (VI.2). For our present choice of $\nu = 0$, this constraint implies the restriction to a one-dimensional compact subspace of the two-dimensional \mathbb{R}^2 :

$$p_0^2 + 4p_0p_1 + 6p_1^2 = 1 . \quad (\text{VI.34})$$

Since such a closed subspace is topologically equivalent to a circle S^1 , one may introduce a circular coordinate (α , say) in order to parameterize both real numbers p_0, p_1 :

$$p_0 = \cos \alpha - \sqrt{2} \sin \alpha \quad (\text{VI.35a})$$

$$p_1 = \frac{\sin \alpha}{\sqrt{2}} . \quad (\text{VI.35b})$$

Indeed, one is easily convinced that the constraint (VI.34) is automatically satisfied by this parametrization. Furthermore, the kinetic energy function $\tilde{\varepsilon}_{\text{kin}}(p_0, p_1)$ (VI.30) becomes now also a function of this angular parameter α , i.e.

$$\tilde{\varepsilon}_{\text{kin}}(p_0, p_1) \Rightarrow \tilde{\varepsilon}_{\text{kin}}(\alpha) = \frac{1}{4} \left(1 + \tilde{T}_1(\alpha) \right) \quad (\text{VI.36a})$$

$$\tilde{T}_1(\alpha) = 2 \sin \alpha \left(\sin \alpha - \sqrt{2} \cos \alpha \right) . \quad (\text{VI.36b})$$

The same arguments do also convert the potential function $\tilde{\varepsilon}_{\text{pot}}(p_0, p_1)$ (VI.31) into a function of α

$$\tilde{\varepsilon}_{\text{pot}}(p_0, p_1) \Rightarrow \tilde{\varepsilon}_{\text{pot}}(\alpha) = \frac{1}{2} \left(1 + \tilde{V}_1(\alpha) \right) \quad (\text{VI.37a})$$

$$\tilde{V}_1(\alpha) = \sin \alpha \left(\frac{1}{2} \sin \alpha + \frac{\sqrt{2}}{4} \cos \alpha \cdot \sin^2 \alpha - \sqrt{2} \cos \alpha - \frac{7}{8} \sin^3 \alpha \right) . \quad (\text{VI.37b})$$

Consequently, the angular dependence of the spectral function $S_\varphi^{[0]}(\alpha)$ (VI.33) must look as follows

$$S_\varphi^{[0]}(p_0, p_1) \Rightarrow S_\varphi^{[0]}(\alpha) = \frac{(1 + \tilde{V}_1(\alpha))^2}{1 + \tilde{T}_1(\alpha)}. \quad (\text{VI.38})$$

This function has been discussed in some detail in ref. [14] (see equation (IV.44) of that reference); and it has been found that there occur two maxima and two minima which then generate four energy values $E_{1a} \dots E_{1d}$ in the following arrangement:

rel. maxima:

$$E_{1a} = -\frac{e^2}{4a_B} \cdot 1 \simeq -6,8029 \dots \text{ [eV]} \quad (\text{VI.39a})$$

$$E_{1b} = -\frac{e^2}{4a_B} \cdot 0,086717499 \dots \simeq -0,590 \text{ [eV]} \quad (\text{VI.39b})$$

rel. minima:

$$E_{1c} = -\frac{e^2}{4a_B} \cdot 1,033319474 \dots \simeq -7,030 \text{ [eV]} \quad (\text{VI.40a})$$

$$E_{1d} = -\frac{e^2}{4a_B} \cdot 1,128194657 \dots \simeq -7,675 \text{ [eV]}. \quad (\text{VI.40b})$$

Here, the first result E_{1a} (VI.39a) is clearly the most striking one, because it agrees *exactly* with both the zero-order approximation ($\alpha = 0$) and the conventional ground-state prediction (I.4), where the latter is commonly considered to be exact within the framework of the generally accepted non-relativistic quantum mechanics. However, the occurrence of two minima and two maxima in the first-order spectrum demands an explanation: From the physical point of view there should occur for $N = 1$ just one maximum and one minimum, corresponding to the groundstate and the first excited state. But evidently the present approximation procedure generates spectral functions with additional *spurious* extremal values which are not reproduced in the next higher approximation steps. Therefore it may appear desirable to get some confidence in the presently used approximation formalism. This is attained by reproducing the above results through a different parametrization of the trial amplitude (**App.H**).

Summarizing the simplified groundstate treatment, one gets a first estimate of the

groundstate energy at $E_{1d} = -7,675$ [eV] (VI.40b) which deviates in an unacceptable way from the conventional prediction $E_{\text{conv}}^{(1)} = -\frac{e^2}{4a_B} \simeq -6,8029$ [eV], (cf. equation (I.4)). However, this does not mean that RST is unable to reproduce the conventional positronium spectrum (I.4). As we will readily see, the spectrum is actually reproduced by the present approximation formalism with sufficient accuracy as far as the *excited* states are concerned. The *groundstate* seems to represent an exceptional situation which must be studied separately.

4. *Excited States*

For the treatment of the excited states one has of course to relax the condition $\nu = 0$ which may be applicable exclusively for the (simplified) groundstate. Or otherwise, if one wishes to stick to $\nu = 0$, one has to further generalize the present trial ansatz (VI.1) in order to work with the more general hydrogen-like wave functions (the latter approximation method has been applied in ref. [14]). However, for the present elaborations, we rely upon the simpler variational ansatz (VI.1) with general ν and integer quantum number l_ϕ of angular momentum (III.21). This approach must generate the same energy spectrum as does the method of the hydrogen-like wave functions in combination with vanishing angular momentum $l_\phi = 0$, provided the angular momentum degeneracy emerges in RST quite analogously to the situation in the conventional theory based upon the Hamiltonian \hat{H} (I.3).

Thus our procedure will be a slight generalization of the precedent treatment of the simplified groundstate; i.e. for parametrizing the general spectral function $S_\phi(\nu, p_0, p_1)$ (VI.27) (with non-zero variational parameter ν) by the S^1 -coordinate α we first have to look for both functions $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.11) and $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ (VI.13) as functions of that new coordinate α , and afterwards one determines the maximal value of the corresponding function $S_\phi(\nu, \alpha)$.

$$S_\phi(\nu, \alpha) = \frac{\varepsilon_{\text{pot}}^2(\nu, \alpha)}{\varepsilon_{\text{kin}}(\nu, \alpha)} . \quad (\text{VI.41})$$

For such a reparametrization by the angle α it is very convenient to first eliminate from both functions $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ and $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ the parameter p_0 as far as possible since its reparametrization is somewhat more complicated than its associate p_1 :

$$p_0 \Rightarrow p_0(\alpha) = \cos \alpha - \sqrt{2(\nu + 1)} \cdot \sin \alpha \quad (\text{VI.42a})$$

$$p_1 \Rightarrow p_1(\alpha) = \frac{\sin \alpha}{\sqrt{2(\nu + 1)}}. \quad (\text{VI.42b})$$

Clearly, this is the generalization of the predecessors (VI.35a)-(VI.35b) for the simplified groundstate ($\nu = 0$); but indeed it guarantees the validity of the more general normalization condition (VI.2). Thus, the kinetic function $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.11) reappears now in terms of the S^1 -coordinate α as

$$\begin{aligned} \varepsilon_{\text{kin}}(\nu, p_0, p_1) \Rightarrow \varepsilon_{\text{kin}}(\nu, \alpha) &= \frac{1}{2\nu(2\nu + 1)} \left[(\nu + 2l_\varphi^2) \cdot \left(\frac{1}{2} - \sqrt{\frac{2}{\nu + 1}} \sin \alpha \cos \alpha \right) \right. \\ &\quad \left. + \sin^2 \alpha \cdot \left(\nu + \frac{l_\varphi^2}{\nu + 1} \right) \right]. \end{aligned} \quad (\text{VI.43})$$

Evidently, this result becomes reduced to the former case $\varepsilon_{\text{kin}}(\nu)$ (III.53) for $\alpha \rightarrow 0$ (i.e. $p_1 \rightarrow 0, p_0 \rightarrow 1$); and it becomes reduced to the simplified groundstate situation $\tilde{\varepsilon}_{\text{kin}}(\alpha)$ (VI.36a)-(VI.36b) for $l_\varphi = 0, \nu \rightarrow 0$.

The next step must consist in looking for the reparametrized numerator $\varepsilon_{\text{pot}}(\nu, \alpha)$, of the spectral function $S_\varphi(\nu, \alpha)$ (VI.41); i.e. we have to elaborate the transition $\varepsilon_{\text{pot}}(\nu, p_0, p_1) \rightarrow \varepsilon_{\text{pot}}(\nu, \alpha)$ where the original potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ is given by equation (VI.13) and the angular parametrization of p_0, p_1 by equations (VI.42a)-(VI.42b). The result then looks as follows:

$$\begin{aligned} \varepsilon_{\text{pot}}(\nu, p_0, p_1) \Rightarrow \varepsilon_{\text{pot}}(\nu, \alpha) &= \varepsilon_{\text{pot}}(\nu) + \left(\varepsilon_2(\nu) + \frac{\varepsilon_4(\nu)}{2(\nu + 1)} \cdot \sin^2 \alpha \right) \cdot \frac{\sin^2 \alpha}{2(\nu + 1)} \\ &\quad + 2 \left(\varepsilon_1(\nu) + \frac{\varepsilon_3(\nu)}{2(\nu + 1)} \cdot \sin^2 \alpha \right) \cdot \left(\frac{\sin 2\alpha}{\sqrt{2(\nu + 1)}} + \cos 2\alpha - 1 \right). \end{aligned} \quad (\text{VI.44})$$

Clearly, this is the generalization to arbitrary ν of the former potential function $\tilde{\varepsilon}_{\text{pot}}(\alpha)$ (VI.37a)-(VI.37b) which in turn is recovered from the present more general result (VI.44)

by putting ν to zero ($\nu \rightarrow 0$). This claim can easily be validated by observing the definition of the auxiliary functions (see also the table in **App.G**)

$$\varepsilon_1(\nu) \doteq \varepsilon_I(\nu) - 2(\nu + 1) \cdot \varepsilon_{\text{pot}}(\nu) \quad (\text{VI.45a})$$

$$\varepsilon_2(\nu) \doteq 4\varepsilon_{II}(\nu) - 16(\nu + 1) \cdot \varepsilon_I(\nu) + [16(\nu + 1)^2 - 4(\nu + 1)(2\nu + 3)] \cdot \varepsilon_{\text{pot}}(\nu) \quad (\text{VI.45b})$$

$$\varepsilon_3(\nu) \doteq \varepsilon_{III}(\nu) - 4(\nu + 1) \cdot \varepsilon_{II}(\nu) + 2(6\nu^2 + 11\nu + 5) \cdot \varepsilon_I(\nu) \quad (\text{VI.45c})$$

$$- 4(2\nu^3 + 5\nu^2 + 4\nu + 1) \cdot \varepsilon_{\text{pot}}(\nu)$$

$$\begin{aligned} \varepsilon_4(\nu) \doteq & \varepsilon_{IV}(\nu) - 8(\nu + 1)(2\nu + 3) \cdot \varepsilon_{II}(\nu) + 32(\nu + 1)^2(2\nu + 3) \cdot \varepsilon_I(\nu) \\ & - 4(\nu + 1)^2(2\nu + 3)(6\nu + 5) \cdot \varepsilon_{\text{pot}}(\nu) \end{aligned} \quad (\text{VI.45d})$$

Thus, putting ν to zero yields

$$\varepsilon_1(0) = -\frac{1}{4} \quad (\text{VI.46a})$$

$$\varepsilon_2(0) = -\frac{3}{2} \quad (\text{VI.46b})$$

$$\varepsilon_3(0) = \frac{1}{8} \quad (\text{VI.46c})$$

$$\varepsilon_4(0) = -\frac{3}{4} \quad (\text{VI.46d})$$

and this simplifies the general $\varepsilon_{\text{pot}}(\nu, \alpha)$ (VI.44) actually down to the former $\tilde{\varepsilon}_{\text{pot}}(\alpha)$ (VI.37a)-(VI.37b).

With both the numerator $\varepsilon_{\text{pot}}(\nu, \alpha)$ and denominator $\varepsilon_{\text{kin}}(\nu, \alpha)$ of the spectral function $S_\phi(\nu, \alpha)$ (VI.41) being known now, one can let search the maximum $S_\phi^{[n]}(*)$ of $S_\phi(\nu, \alpha)$ by means of an appropriate numerical program and finally can then tabulate the corresponding positronium spectrum $\mathbb{E}_\phi^{[n]}$

$$\mathbb{E}_\phi^{[n]} = -\frac{e^2}{4a_B} \cdot S_\phi^{[n]}(*) \quad (\text{VI.47a})$$

$$S_\phi^{[n]}(*) := S_\phi(\nu_*^{[n]}, p_*^{[n]}) , \quad (\text{VI.47b})$$

see **table 3** below.

As a check for the correct working of the program, one can alternatively determine the energy spectrum also in the reparametrized form (H.26a)-(H.26b) which must identically reproduce the spectrum due to the present form (VI.47a)-(VI.47b).

n_P $(= lp + 1)$	$E_{\text{conv}}^{(n)}$ (I.4)	$\mathbb{E}_p^{[n]}$ (VI.47a)-(VI.47b)	$\nu_*^{[n]}$	$p_*^{[n]}$	$\Delta_\varphi(\nu_*^{[n]})$ (VI.48)
1	-6.80290	-7.67499	0.00000	0.56525	-12.82
2	-1.70072	-1.56251	1.25829	0.67798	8.13
3	-0.75588	-0.67055	3.46267	-0.04753	11.29
4	-0.42518	-0.37411	5.42898	-0.03560	12.01
5	-0.27212	-0.23925	7.52949	-0.02837	12.08
6	-0.18897	-0.16647	9.74795	-0.02351	11.91
7	-0.13883	-0.12267	12.07237	-0.02001	11.65
8	-0.10630	-0.09423	14.49351	-0.01738	11.35
9	-0.08399	-0.07470	17.00395	-0.01532	11.06
10	-0.06803	-0.06070	19.59761	-0.01367	10.77
11	-0.05622	-0.05033	22.26932	-0.01232	10.49
12	-0.04724	-0.04241	25.01475	-0.01120	10.22
13	-0.04025	-0.03624	27.82998	-0.01025	9.97
14	-0.03471	-0.03133	30.71171	-0.00944	9.74
15	-0.03024	-0.02736	33.65704	-0.00874	9.51

Table 3: Improved RST predictions (Spherical Symmetry)

The improved RST predictions $\mathbb{E}_\varphi^{[n]}$ (VI.47a) (spherically symmetric approximation) do differ essentially from their conventional counterparts $E_{\text{conv}}^{(n)}$ (I.4) if compared to the corresponding “anisotropic” improvements of **table 2** (p. 77). Defining here the deviation $\bar{\Delta}_{[\varphi]}$ quite analogously to the former cases $\bar{\Delta}_{[T]}$ (III.58) and $\bar{\Delta}_{\{T\}}$ (V.44) as

$$\bar{\Delta}_{[\varphi]} = \frac{1}{14} \sum_{n=2}^{14} \left(\frac{E_{\text{conv}}^{(n)} - \mathbb{E}_\varphi^{[n]}}{E_{\text{conv}}^{(n)}} \right) = \frac{1}{14} \sum_{n=2}^{14} \Delta_\varphi(\nu_*^{[n]}) , \quad (\text{VI.48})$$

one finds for the present improvement of the spherically symmetric type

$$\bar{\Delta}_{[\phi]} = 10,7\% \quad (\text{VI.49})$$

This is an irrelevant improvement in comparison to the analogous average of 10,9% due to the simplest approximation (**table 1**, $2 \leq n_\phi \leq 15$). Observe also that for the ground-state ($n_\phi = 1$) one finds $\nu_*^{[1]} \simeq 0$ which is preliminarily assumed for the sake of simplicity in order to exemplify our general approximation scheme, see the precedent **Section VI.3**. Through this fortuitous agreement, the former groundstate prediction E_{1d} (VI.40b) is practically identical with the result $E_\phi^{[1]}$ of the present more rigorous calculation (first line, $n_\phi = 1$).

VII Conclusion

The present results may give to us now a hint at the direction for searching further improvements. It is true, both higher approximations (i.e. the “anisotropic” one of **table 2** and the “spherically symmetric” one of **table 3**) yield certain improvements in the sense that the corresponding RST predictions do better approach the predictions $E_{\text{conv}}^{(n)}$ (I.4) of the conventional theory. However, the improvement of the spherically symmetric kind (**table 3**) are inconsiderable because they amount to merely some 0,2 percent. Thus the conclusion is that the original results of the spherically symmetric type (**table 1**) do already exhaust the possibilities of this symmetry. But the “anisotropic” improvements (**table 2**) do reduce the RST deviations (from the conventional predictions) by some 50% in the range $2 \leq n_\phi \leq 15$. Therefore one expects that the next higher approximation step of the anisotropic type (i.e. the regard of the radial auxiliary potential $\{^{\text{p}}\}A^V(r)$ in the expansion (V.3)) will show a further clear step of the RST predictions towards the conventional energy spectrum (I.4). Here, the regard of the anisotropy can not be restricted to the interaction potential ${}^{\text{p}}A_0$ alone but must refer also to the wave functions themselves. More concretely, this means that the product ansatz (III.17a)-(III.17b) for the wave amplitudes must receive some generalization. Taking all these results together, it seems that the conventional levels (I.4) play the part of a lower bound for the successively higher RST approximations. In any case, further clarification of this question must be left to a more extensive investigation.

Appendix A: *Spherically Symmetric Potential*

The spherically symmetric approximation is defined by assuming the electric interaction potential ${}^{(p)}A_0(\vec{r})$ (II.30) to be SO(3) symmetric, cf. equation (III.1). The *principle of minimal energy* (II.40) then yields the Poisson equation (III.36) for the symmetric potential $[p]A_0(r)$ which may be recast to the following dimensionless form

$$\frac{d^2\tilde{a}_\nu(y)}{dy^2} + \frac{2}{y} \frac{d\tilde{a}_\nu(y)}{dy} = -e^{-y} \frac{y^{2\nu-1}}{\Gamma(2\nu+2)} \quad (A.1)$$

$$(y \doteq 2\beta r) ,$$

provided the original potential $[p]A_0(r)$ (III.1) due to the trial amplitude $\tilde{\Phi}(r)$ is rescaled as follows

$$[p]A_0(r) \doteq 2\beta\alpha_s \cdot \tilde{a}_\nu(y) , \quad (A.2)$$

and similarly for the trial function $\tilde{\Phi}(r)$ (III.50)

$$\tilde{\Phi}(r) = \sqrt{\frac{2}{\pi}} \cdot \frac{2\beta}{\sqrt{\Gamma(2\nu+2)}} \tilde{\Phi}_\nu(y) \quad (A.3a)$$

$$\tilde{\Phi}_\nu(y) \doteq y^\nu \cdot e^{-\frac{y}{2}} . \quad (A.3b)$$

The solutions $\tilde{a}_\nu(y)$ of the dimensionless Poisson equation (A.1) can be represented for integer values of 2ν in form of a recurrence formula:

$$\tilde{a}_{\nu+\frac{1}{2}}(y) = \tilde{a}_\nu(y) - \frac{e^{-y}}{(2\nu+2)(2\nu+1)} \cdot \sum_{n=0}^{2\nu} \frac{y^n}{n!} , \quad (A.4)$$

with the lowest-order potential $\tilde{a}_0(y)$ for $\nu = 0$ being given by

$$\tilde{a}_0(y) = \frac{1}{y} (1 - e^{-y}) . \quad (A.5)$$

Thus, the lowest-order potentials (i.e. for $\nu = 0, \frac{1}{2}, 1, \frac{3}{2}$) are found to be of the following shape

$$\tilde{a}_{\frac{1}{2}}(y) = \tilde{a}_0(y) - \frac{e^{-y}}{2} = \frac{1}{y} \left\{ 1 - e^{-y} \left(1 + \frac{y}{2} \right) \right\} \quad (\text{A.6a})$$

$$\tilde{a}_1(y) = \tilde{a}_{\frac{1}{2}}(y) - \frac{e^{-y}}{6} (1+y) = \frac{1}{y} \left\{ 1 - e^{-y} \left(1 + \frac{2y}{3} + \frac{y^2}{6} \right) \right\} , \quad (\text{A.6b})$$

$$\tilde{a}_{\frac{3}{2}}(y) = \tilde{a}_1(y) - \frac{e^{-y}}{12} \left(1 + y + \frac{y^2}{2} \right) = \frac{1}{y} \left\{ 1 - e^{-y} \left(1 + \frac{3}{4}y + \frac{1}{4}y^2 + \frac{1}{24}y^3 \right) \right\} , \quad (\text{A.6c})$$

see fig. A.I below for a sketch of these lowest-order potentials. For general (but still integer) values of 2ν the dimensionless potential $\tilde{a}_\nu(y)$ (A.4) looks as follows:

$$\tilde{a}_\nu(y) = \frac{1}{y} \left(1 - e^{-y} \cdot \sum_{n=0}^{2\nu} \frac{2\nu+1-n}{2\nu+1} \cdot \frac{y^n}{n!} \right) . \quad (\text{A.7})$$

Here it must be stressed that such a potential $\tilde{a}_\nu(y)$ does actually exist for any real-valued $\nu (> -\frac{1}{2})$, where the general expression for this situation is then given by an *infinite* sum

$$\tilde{a}_\nu(y) = \frac{1}{2\nu+1} \left(1 - e^{-y} \cdot \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu+2+n)} y^{2\nu+n} \right) , \quad (\text{A.8})$$

see appendix D of ref. [11].

The value $\tilde{a}_\nu(0)$ of the potentials $\tilde{a}_\nu(y)$ (A.5)-(A.6c) at the origin ($y = 0$) is easily found by expanding the exponential function e^{-y} in the usual way which then yields

$$\tilde{a}_0(0) = 1 \quad (\text{A.9a})$$

$$\tilde{a}_{\frac{1}{2}}(0) = \frac{1}{2} \quad (\text{A.9b})$$

$$\tilde{a}_1(0) = \frac{1}{3} \quad (\text{A.9c})$$

$$\tilde{a}_{\frac{3}{2}}(0) = \frac{1}{4} , \quad (\text{A.9d})$$

see also the sketch A.I of potentials $\tilde{a}_\nu(y)$ below. Obviously the general case is given by

$$\tilde{a}_\nu(0) = \frac{1}{2\nu+1} ; \quad (\text{A.10})$$

and this result does hold for any real-valued power $\nu > -\frac{1}{2}$. Indeed, this claim can easily be verified by exploiting the general shape of the solution of the Poisson equation (A.1)

$$\tilde{a}_\nu(y) = \frac{1}{4\pi \cdot \Gamma(2\nu + 2)} \int d^3\vec{y}' \frac{e^{-y'} \cdot y'^{2\nu-1}}{\|\vec{y} - \vec{y}'\|} \quad (\text{A.11})$$

which satisfies also the usual boundary condition at infinity ($y \rightarrow \infty$)

$$\lim_{y \rightarrow \infty} \tilde{a}_\nu(y) = \frac{1}{y} \quad \forall \nu . \quad (\text{A.12})$$

In terms of the original potential ${}^{[\text{p}]}A_0(r)$ (A.2) this boundary condition (A.12) yields just the well-known Coulomb form

$$\lim_{r \rightarrow \infty} {}^{[\text{p}]}A_0(r) = \frac{\alpha_s}{r} \quad (\text{A.13})$$

which thus is found to be the asymptotic limit form for all potentials ${}^{[\text{p}]}A_0(r)$ being due to the class of trial functions $\tilde{\Phi}(r)$ (III.50), irrespective of the special value of ν .

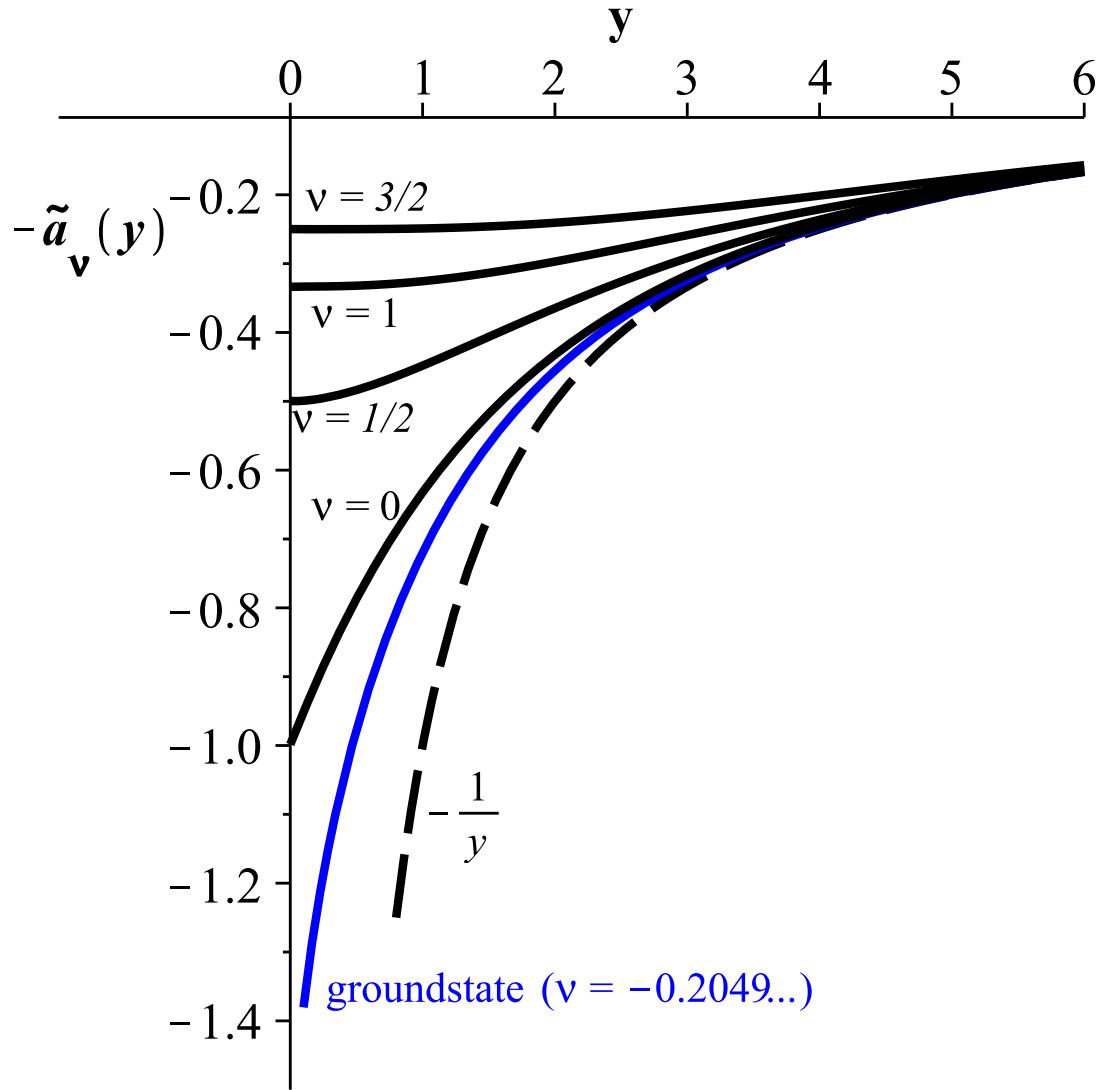


Fig. A.I: Spherically Symmetric Potentials (A.5)-(A.6c)

The potentials $\tilde{a}_\nu(y)$ (A.8) are finite at the origin ($y = 0$), cf. (A.10), and approach the Coulomb potential ($\sim \frac{1}{y}$) for $y \rightarrow \infty$, cf. (A.12). For the excited states the parameter ν is positive (see the **table 1** on p. 44) and therefore the potentials $\tilde{a}_\nu(y)$ have vanishing derivative at the origin ($y = 0$), but for the groundstate ($\nu_* = -0,2049\dots$) the derivative becomes infinite, see equation (A.20) below.

The fact that the spherically symmetric potentials ${}^{[p]}A_0(r)$ are finite at the origin ($r = 0$) does of course not mean that the corresponding field strength \vec{E}_p felt by the electron

$$\vec{E}_p(\vec{r}) = \vec{\nabla} {}^{[p]}A_0(r) = \frac{d {}^{[p]}A_0(r)}{dr} \vec{e}_r \quad (\text{A.14})$$

is in any case a regular vector field for $r \rightarrow 0$. Indeed, introducing the dimensionless form $\tilde{e}_\nu(y)$ of the radial component ${}^{[p]}E_r(r)$

$$\vec{E}_p(\vec{r}) = {}^{[p]}E_r(r)\vec{e}_r \quad (\text{A.15})$$

through

$${}^{[p]}E_r(r) = \frac{d {}^{[p]}A_0(r)}{dr} \doteq (2\beta)^2 \alpha_s \tilde{e}_\nu(y) , \quad (\text{A.16})$$

one arrives at the following link of (dimensionless) potentials $\tilde{a}_\nu(y)$ and field strengths $\tilde{e}_\nu(y)$:

$$\tilde{e}_\nu(y) = \frac{d\tilde{a}_\nu(y)}{dy} . \quad (\text{A.17})$$

But since the spherically symmetric potentials $\tilde{a}_\nu(y)$ are explicitly known both for integer 2ν (A.7) and general ν (A.8), the field strengths $\tilde{e}_\nu(y)$ are also known, e.g. for integer 2ν :

$$\tilde{e}_\nu(y) = -\frac{1}{y^2} \left(1 - e^{-y} \cdot \sum_{n=0}^{2\nu+1} \frac{y^n}{n!} \right) , \quad (\text{A.18})$$

or similarly for general ν

$$\tilde{e}_\nu(y) = -e^{-y} \cdot \sum_{n=0}^{\infty} \frac{y^{2\nu+n}}{\Gamma(2\nu+3+n)} . \quad (\text{A.19})$$

From this latter result it is now easily seen that the field strength does behave at the origin as follows:

$$\lim_{y \rightarrow 0} \tilde{e}_\nu(y) = -\lim_{y \rightarrow 0} \frac{y^{2\nu}}{\Gamma(2\nu+3)} = \begin{cases} -\infty , & \nu < 0 \\ -\frac{1}{2} , & \nu = 0 \\ 0 , & \nu > 0 . \end{cases} \quad (\text{A.20})$$

This says that the field strength $\vec{E}_p(\vec{r})$ (A.14) is a non-singular unique vector field only for $\nu > 0$, see the figure A.II below. Thus it is only for the groundstate $\nu \simeq -0, 2$ that the electric field strength turns out to be singular at the origin ($y = 0$). Observe also that (for all ν) the field strength $\tilde{e}_\nu(y)$ adopts the Coulomb form (broken line) at infinity, i.e.

$$\lim_{y \rightarrow \infty} \tilde{e}_\nu(y) = -\frac{1}{y^2}, \quad \forall \nu \quad (\text{A.21})$$

quite similarly as for the potential $\tilde{a}_\nu(y)$ (A.12).

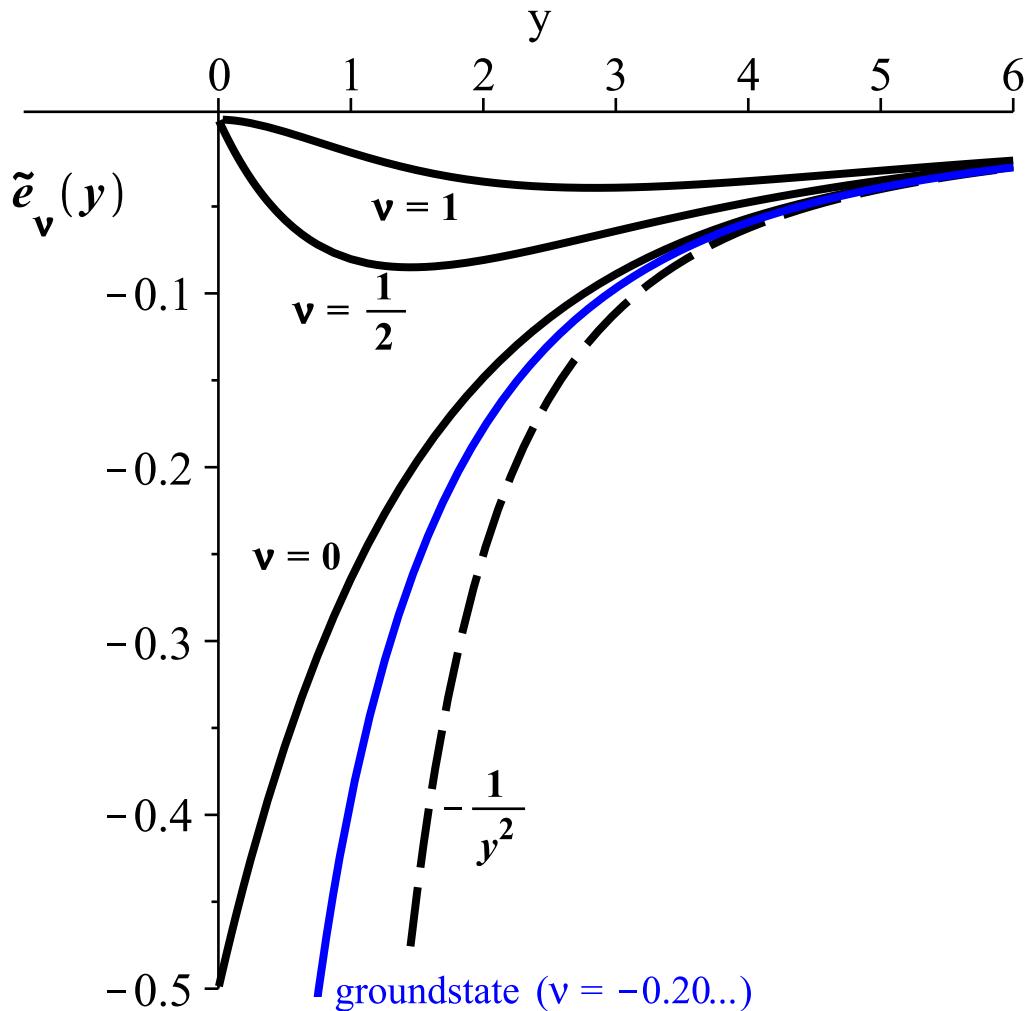


Fig. A.II: *Electric Field Strength $\tilde{e}_\nu(y)$ (A.18)-(A.19)*

The electric field strength $\tilde{e}_\nu(y)$ is non-singular only for the excited states which have positive variational parameter ν . However, for the groundstate ($\nu \simeq -0.2$) the field strength becomes singular, albeit less singular than the Coulomb field ($\sim -\frac{1}{y^2}$). This guarantees that the energy content $E_R^{(e)}$ (II.36) of the gauge field remains finite.

In the present context of positronium binding energy, the essential point refers now to the value of the non-relativistic energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) upon the class of trial functions $\tilde{\Phi}(r)$ (III.50). Indeed, the desired approximate spectrum of binding energies emerges as the set of extremal values of $\tilde{\mathbb{E}}_{[\Phi]}$ on that chosen class of trial functions $\tilde{\Phi}(r)$ (III.50). More concretely, the value of $\tilde{\mathbb{E}}_{[\Phi]}$ upon that class yields a function $\mathbb{E}^{[IV]}(\beta, \nu)$ of the two variational parameters β and ν which looks as follows [11]:

$$\begin{aligned}\mathbb{E}^{[IV]}(\beta, \nu) &= \frac{e^2}{a_B} \left[(2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (2a_B \beta) \cdot \varepsilon_{\text{pot}}(\nu) \right] \\ &\quad \left(a_B \doteq \frac{\hbar^2}{Me^2} \right).\end{aligned}\tag{A.22}$$

The extremalization procedure due to the principle of minimal energy (II.40) requires now to look for the stationary points of this function $\mathbb{E}^{[IV]}(\beta, \nu)$:

$$\frac{\partial \mathbb{E}^{[IV]}(\beta, \nu)}{\partial \beta} = 0\tag{A.23a}$$

$$\frac{\partial \mathbb{E}^{[IV]}(\beta, \nu)}{\partial \nu} = 0.\tag{A.23b}$$

It is easy to see that these two requirements can be reduced to the one requirement

$$\frac{\partial \mathbb{E}_T(\nu)}{\partial \nu} = 0\tag{A.24}$$

with the reduced energy function $\mathbb{E}_T(\nu)$ being defined through [11]

$$\mathbb{E}_T(\nu) \doteq -\frac{e^2}{4a_B} \cdot S_\varphi(\nu).\tag{A.25}$$

The *spectral function* $S_\varphi(\nu)$ emerging here is itself defined in terms of the variational parameter ν through

$$S_\varphi(\nu) \doteq \frac{\varepsilon_{\text{pot}}^2(\nu)}{\varepsilon_{\text{kin}}(\nu)},\tag{A.26}$$

with the *kinetic function* $\varepsilon_{\text{kin}}(\nu)$ depending upon the variational parameter ν and upon the angular momentum quantum number l_φ (III.33) in the following way [11]

$$\varepsilon_{\text{kin}}(\nu) = \frac{1}{2\nu + 1} \left(\frac{1}{4} + \frac{l_\varphi^2}{2\nu} \right).\tag{A.27}$$

Furthermore, the *potential function* $\varepsilon_{\text{pot}}(\nu)$ is found to be somewhat more complicated but can be represented by virtue of the *Poisson identity* in two equivalent ways [11]

$$\begin{aligned}\varepsilon_{\text{pot}}(\nu) &= \frac{1}{2^{4\nu+3}} \sum_{m,n=0}^{\infty} \frac{1}{2^{m+n}} \cdot \frac{\Gamma(4\nu + 3 + m + n)}{\Gamma(2\nu + 3 + m) \cdot \Gamma(2\nu + 3 + n)} \\ &= \frac{1}{2\nu + 1} \left(1 - \frac{1}{2^{4\nu+2}} \cdot \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu + 2 + n)}{\Gamma(2\nu + 2) \cdot \Gamma(2\nu + 2 + n)} \right).\end{aligned}\quad (\text{A.28})$$

It follows from the present results in combination with the *principle of minimal energy* (II.40) that the non-relativistic positronium spectrum may be obtained by looking for the stationary points of the spectral function $S_\varphi(\nu)$ (A.26) for any quantum number l_φ . But since our trial function $\tilde{\Phi}(r)$ (III.50) is too simple in order to get the whole spectrum of excited states due to the one chosen l_φ , one will obtain in this way merely the “ground-state” for any l_φ , cf. figure 2 of ref. [11]. The result of this extremalization procedure is presented by **table 1** on page 44.

Appendix B: *Auxiliary Potentials* $\{^p\!A_I$, $\{^p\!A_{III}$, $\{^p\!A_V$ *for general ν*

For an estimate of the radial auxiliary potentials (IV.11a)-(IV.11e) due to *general* ν it is most convenient to first recast these potentials to a dimensionless form, quite similarly as it was done for the spherically symmetric approximation $[^p\!A_0(r)$, cf. equation (A.2); i. e. we put

$${}^{(I)}\tilde{a}(y) \doteq (2\beta\alpha_s)^{-1} \cdot \{^p\!A_I(r) = \int_0^\infty dy' \frac{y'}{[y^2 + y'^2]^{\frac{1}{2}}} \cdot \tilde{\Phi}^2(y') \quad (\text{B.1a})$$

$${}^{(III)}\tilde{a}(y) \doteq (2\beta\alpha_s)^{-1} \cdot \{^p\!A_{III}(r) = y^2 \cdot \int_0^\infty dy' \frac{y'^3}{[y^2 + y'^2]^{\frac{5}{2}}} \cdot \tilde{\Phi}^2(y') \quad (\text{B.1b})$$

$${}^{(V)}\tilde{a}(y) \doteq (2\beta\alpha_s)^{-1} \cdot \{^p\!A_V(r) = y^4 \cdot \int_0^\infty dy' \frac{y'^5}{[y^2 + y'^2]^{\frac{9}{2}}} \cdot \tilde{\Phi}^2(y') \quad (\text{B.1c})$$

⋮

$$\left(\tilde{\Phi}(y) \doteq \frac{\tilde{\Phi}(r)}{2\beta}, \quad y \doteq 2\beta r \right).$$

The differential links (IV.20)-(IV.21) read now in this dimensionless form

$${}^{(III)}\tilde{a}(y) = -\frac{1}{3} y \frac{d^2}{dy^2} \left(y \cdot {}^{(I)}\tilde{a}(y) \right) \quad (\text{B.2a})$$

$${}^{(V)}\tilde{a}(y) = -\frac{1}{35} y^3 \frac{d}{dy} \left[\frac{1}{y^4} \frac{d}{dy} \left(y^3 \cdot {}^{(III)}\tilde{a}(y) \right) \right] \quad (\text{B.2b})$$

⋮

For a treatment of the excited states it is necessary to admit the variational parameter ν in the trial amplitude $\tilde{\Phi}(r)$ (III.50) to adopt quite general (real) values, not only the special value $\nu = 0$ which is adopted in **Sect. IV.2** for the simplified treatment of the groundstate. For such a more general situation, one may still take as the starting potential

$\{^p\}A_I(r)$ again the spherically symmetric potential $[^p]A_0(r)$ which obeys the spherically symmetric Poisson equation (III.36) but now with non-zero ν :

$$\frac{1}{(2\beta)^2} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) [^p]A_0(r) = -\frac{2\beta\alpha_s}{\Gamma(2\nu+2)} \cdot (2\beta r)^{2\nu-1} e^{-2\beta r}, \quad (\text{B.3})$$

cf. also the dimensionless form (A.1) of this Poisson equation and its solution (A.8). Thus our starting potential $(^0)\tilde{a}_\nu(y)$ is now just that spherically symmetric approximation (A.8); i. e. we put

$$(^0)\tilde{a}_\nu(y) \equiv \frac{2}{\pi} (2\beta\alpha_s)^{-1} [^p]A_0(r) = \frac{2}{\pi} \frac{1}{2\nu+1} \left(1 - e^{-y} \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu+2+n)} y^{2\nu+n} \right). \quad (\text{B.4})$$

For integer values of 2ν (i. e. $\nu = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots$) this starting potential appears as a finite sum, namely [11]

$$(^0)\tilde{a}_\nu(y) = \frac{2}{\pi} \frac{1}{y} \left(1 - e^{-y} \sum_{n=0}^{2\nu} \frac{2\nu+1-n}{2\nu+1} \cdot \frac{y^n}{n!} \right). \quad (\text{B.5})$$

Clearly, for $\nu = 0$ one recovers here the former starting potential $\{^p\}A_I(r)$ (IV.25).

But now that the more general starting potential $(^0)\tilde{a}_\nu(y)$ has been fixed, one can use it in order to calculate the associated third auxiliary potential $(^{III})\tilde{a}_\nu(y)$ (B.2a):

$$(^{III})\tilde{a}_\nu(y) = -\frac{1}{3} y \frac{d^2}{dy^2} \left(y \cdot (^0)\tilde{a}_\nu(y) \right) = \frac{2}{3\pi} \frac{y^{2\nu+1} e^{-y}}{\Gamma(2\nu+2)}. \quad (\text{B.6})$$

As a consistency check, one puts here $\nu = 0$ which yields

$$(^{III})\tilde{a}_0(y) = \frac{2}{3\pi} y e^{-y} = \frac{2}{3\pi} (2\beta r) e^{-2\beta r}, \quad (\text{B.7})$$

and thus the third radial potential $\{^p\}A_{III}(r)$ for $\nu = 0$ becomes

$$\{^p\}A_{III}(r) = 2\beta\alpha_s \cdot (^{III})\tilde{a}_0(y) = \frac{8}{3\pi} \alpha_s \beta^2 r e^{-2\beta r} \quad (\text{B.8})$$

which is nothing else than the former result (IV.26a) being used for the simplified treatment of the groundstate. Once the third auxiliary potential $(^{III})\tilde{a}_\nu(y)$ is known, cf. (B.6),

one can proceed to calculate by means of it the corresponding fifth auxiliary potential $(^V)\tilde{a}_\nu(y)$ (B.2b):

$$\begin{aligned} (^V)\tilde{a}_\nu(y) &= -\frac{1}{35}y^3 \frac{d}{dy} \left[\frac{1}{y^4} \frac{d}{dy} \left(y^3 \cdot (^{III})\tilde{a}_\nu(y) \right) \right] \\ &= -\frac{2}{105\pi} \frac{1}{\Gamma(2\nu+2)} e^{-y} \left\{ y^{2\nu+3} - 4(\nu+1)y^{2\nu+2} + 2(\nu+2)(2\nu-1)y^{2\nu+1} \right\}. \end{aligned} \quad (\text{B.9})$$

The consistency check for $\nu = 0$ yields here

$$(^V)\tilde{a}_0(y) = -\frac{16}{105\pi} e^{-y} \left\{ \frac{y^3}{8} - \frac{1}{2}y^2 - \frac{1}{2}y \right\}, \quad (\text{B.10})$$

i. e. for the potential $\{^p\}A_V(r)$ due to $\nu = 0$ one obtains

$$\{^p\}A_V(r) = 2\beta\alpha_s (^V)\tilde{a}_0(y) = -\frac{16}{105\pi} (2\beta\alpha_s) e^{-2\beta r} \left\{ \frac{(2\beta r)^3}{8} - \frac{1}{2}(2\beta r)^2 - \frac{1}{2}(2\beta r) \right\} \quad (\text{B.11})$$

and this again is just the former result (IV.26b) for the simplified groundstate.

Furthermore it is also rather obvious that it is the auxiliary potential of lowest order, i. e. $(^0)\tilde{a}_\nu(y)$ (B.4), which obeys the Coulomb-like boundary condition (IV.18) at infinity ($(^0)\tilde{a}_\nu(y) \rightarrow \frac{2}{\pi} \cdot \frac{1}{y}$) whereas all auxiliary potentials of higher order (e. g. $(^{III})\tilde{a}_\nu(y)$ (B.6) and $(^V)\tilde{a}_\nu(y)$ (B.9)) tend to zero more rapidly than the Coulomb potential ($\sim \frac{1}{y}$). Similarly, the boundary conditions at the origin ($y = 0 \Leftrightarrow r = 0$) are also satisfied: the higher-order potentials such as $(^{III})\tilde{a}_\nu(y)$ (B.6) and $(^V)\tilde{a}_\nu(y)$ (B.9) do actually vanish at the origin ($y = 0$) and thus validate the boundary conditions (IV.16). On the other hand, it is only the auxiliary potential of lowest order (i. e. $(^0)\tilde{a}_\nu(y)$ (B.4)) which adopts the required non-zero values (IV.13) at the origin ($y = 0$).

Summarizing, the expansion (IV.9) generates a hierarchical set of radial auxiliary potentials (IV.11a)-(IV.11e) etc. of ever decreasing magnitude; for the three lowest-order potentials $(^0)\tilde{a}_\nu(y)$ (B.5), $(^{III})\tilde{a}_\nu(y)$ (B.6) and $(^V)\tilde{a}_\nu(y)$ (B.9), see the figure B.I below. With increasing order of this “anisotropy expansion” the deviation of the corresponding electrostatic potential $\{^p\}A_0(r, \vartheta)$ (IV.9) from the exact potential (IV.5) becomes reduced step by step. In the present context, the importance of such an expansion refers to the

gauge field energy $E_R^{(e)}$ (II.36) which undergoes a corresponding expansion with respect to the magnitude of the anisotropy and thus provides us with an estimate of the relative weight of the anisotropic terms (compare, e.g., the “anisotropic” groundstate energy (IV.45) to its “isotropic” counterpart (IV.46), where a deviation of only 0.4% arises). Though the treatment of the groundstate ($\nu = 0$) on the basis of the present anisotropic correction $\{^p\}A_{III}(r)$ (B.8) appears to be meaningful, the generalization to the excited states $\nu > 0$ turns out to be unacceptable (see **App. C**).

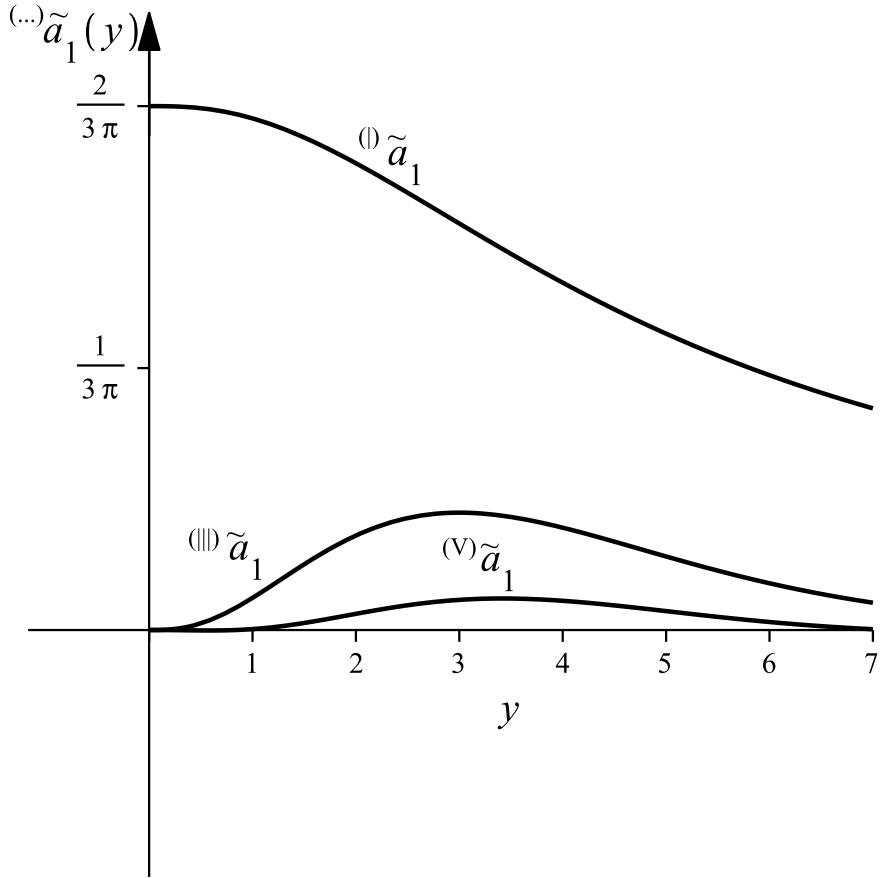


Fig. B.I Radial Auxiliary Potentials $\{I\}\tilde{a}_1$, $\{III\}\tilde{a}_1$, $\{V\}\tilde{a}_1$ (B.5), (B.6) and (B.9)

The hierarchy of magnitudes of the potentials $\{I\}\tilde{a}_\nu(y)$, $\{III\}\tilde{a}_\nu(y)$, $\{V\}\tilde{a}_\nu(y)$, ... persists also for $\nu > 0$ (here $\nu = 1$) similarly as shown for $\nu = 0$ by **Fig. IV.A**. Nevertheless the associated series expansion (IV.9) of the anisotropic potential $\{^p\}A_0(r, \vartheta)$ fails to describe the excited states correctly, see **App. C**.

Appendix C:

Failure of the Expansion (IV.9) for the Excited States ($\nu > 0$)

As plausible as the result of the simplified groundstate ($\nu = 0$) may appear (see the discussion below (IV.46)), this way of dealing with the anisotropic corrections cannot be transferred to the excited states! Indeed, we will readily see that the energy predictions of the excited states would come out in an unacceptable magnitude. Since the simplified groundstate discussion is based upon the “anisotropy expansion” (IV.9), this expansion must be afflicted with a serious deficiency, at least as far as the excited states are concerned. Therefore, an improved expansion is presented in **Sect. V**, but for the sake of completeness we will subsequently work out the reduced energy function $\tilde{\mathbb{E}}_*(\nu)$ due to the (rejectable) series expansion (IV.9), in order to see more clearly what is going wrong with this expansion.

To this end, we compute the corresponding energy function $\tilde{\mathbb{E}}_\Phi(\beta, \nu)$ which is to be understood as the generalization of the groundstate function $\tilde{\mathbb{E}}_\Phi(\beta)$ (IV.43), such that

$$\tilde{\mathbb{E}}_\Phi(\beta) = \tilde{\mathbb{E}}_\Phi(\beta, \nu) \Big|_{\nu=0} . \quad (\text{C.1})$$

Here it is convenient to scale off the atomic energy unit (a. u.) by introducing the spectral function $S_\wp^{\{*\}}$ through

$$\begin{aligned} \mathbb{E}_*(\nu) &\doteq -\frac{e^2}{4a_B} S_\wp^{\{*\}}(\nu) \\ \left(\frac{e^2}{4a_B} = 6.8029\dots \text{ [eV]} \right), \end{aligned} \quad (\text{C.2})$$

so that we are left with the problem to elaborate this spectral function $S_\wp^{\{*\}}(\nu)$ for general ν . Clearly, its extremal values will then yield the wanted energy spectrum of positronium (though to be rejected).

Fortunately, it is possible to explicitly calculate that spectral function $S_\varphi^{(*)}(\nu)$ (C.2) for *integer* 2ν . More concretely, the general gauge field energy $E_R^{(e)}$ (II.36) appears now in terms of the dimensionless auxiliary potentials ${}^{(I)}\tilde{a}_\nu(y)$ (B.4) and ${}^{(III)}\tilde{a}_\nu(y)$ (B.6) as a sum of three terms, cf. equation (IV.32), with each of the three terms being found to appear in the following form:

$$E_{I}^{\{e\}} \doteq -\hbar c (2\beta\alpha_s) \left(\frac{\pi}{2}\right)^2 \int_0^\infty dy y^2 \left(\frac{d {}^{(I)}\tilde{a}_\nu(y)}{dy}\right)^2 \doteq -2\beta e^2 \cdot {}^{(I)}\varepsilon_{\text{pot}}(\nu) \quad (\text{C.3a})$$

$$E_{II}^{\{e\}} \doteq -\hbar c (2\beta\alpha_s) \left(\frac{\pi}{2}\right)^2 \int_0^\infty dy y^2 \frac{d {}^{(I)}\tilde{a}_\nu(y)}{dy} \cdot \frac{d {}^{(III)}\tilde{a}_\nu(y)}{dy} \doteq -2\beta e^2 \cdot {}^{(II)}\varepsilon_{\text{pot}}(\nu) \quad (\text{C.3b})$$

$$E_{III}^{\{e\}} \doteq -\hbar c (2\beta\alpha_s) \frac{3\pi^2}{160} \int_0^\infty dy y^2 \left\{ \frac{7}{2} \left(\frac{d {}^{(III)}\tilde{a}_\nu(y)}{dy} \right)^2 + \left[\frac{{}^{(III)}\tilde{a}_\nu(y)}{y} \right]^2 \right\} \doteq -2\beta e^2 \cdot {}^{(III)}\varepsilon_{\text{pot}}(\nu) . \quad (\text{C.3c})$$

But since the radial auxiliary potentials ${}^{(I)}\tilde{a}_\nu(y)$ and ${}^{(III)}\tilde{a}_\nu(y)$ are explicitly known, cf. (B.4)-(B.6), one can calculate here also explicitly the three auxiliary potential functions ${}^{(I)}\varepsilon_{\text{pot}}(\nu)$, ${}^{(II)}\varepsilon_{\text{pot}}(\nu)$ and ${}^{(III)}\varepsilon_{\text{pot}}(\nu)$ for general ν . The result is

$${}^{(I)}\varepsilon_{\text{pot}}(\nu) \equiv \varepsilon_{\text{pot}}(\nu) , \quad \text{cf. (A.28)} \quad (\text{C.4a})$$

$${}^{(II)}\varepsilon_{\text{pot}}(\nu) = \frac{1}{4! 2^{4\nu}} \cdot \frac{\Gamma(4\nu+3)}{\Gamma(2\nu+2)^2} \quad (\text{C.4b})$$

$${}^{(III)}\varepsilon_{\text{pot}}(\nu) = \frac{9+7\nu}{1920} \cdot \frac{\Gamma(4\nu+3)}{2^{4\nu} \cdot \Gamma(2\nu+2)^2} . \quad (\text{C.4c})$$

These three terms add then up to the total “anisotropic” gauge field energy $E_R^{\{e\}}$

$$E_R^{\{e\}} = E_I^{\{e\}} + E_{II}^{\{e\}} + E_{III}^{\{e\}} \doteq -\hbar c (2\beta\alpha_s) \cdot \varepsilon_R^{\{e\}}(\nu) \quad (\text{C.5})$$

where the “anisotropic” potential function $\varepsilon_R^{\{e\}}(\nu)$ is evidently given by

$$\varepsilon_R^{\{e\}}(\nu) \doteq {}^{(I)}\varepsilon_{\text{pot}}(\nu) + {}^{(II)}\varepsilon_{\text{pot}}(\nu) + {}^{(III)}\varepsilon_{\text{pot}}(\nu) . \quad (\text{C.6})$$

Obviously, the present gauge field energy $E_R^{\{e\}}$ (C.5) with (C.4a)-(C.4c) is nothing else than the generalization of the anisotropic groundstate result $E_R^{\{e\}}$ (IV.32)-(IV.33c) to the

excited states. Observe also that the Poisson identity $\tilde{N}_G^{(e)} \equiv 0$ (cf. (IV.38)) is obeyed strictly for the spherically symmetric approximation, but this identity is of course *not* obeyed by the present anisotropic approximation procedure, neither for the groundstate nor for the excited states!

Therefore we have to calculate now the non-relativistic version $\tilde{M}^{\{e\}}c^2$ of the (relativistic) mass equivalent $\tilde{M}^{(e)}c^2$ (II.37) in order to build up again the constraint term $\tilde{N}_G^{(e)}$ (IV.38)-(IV.39), but now for general values of the variational parameter ν . This means that for the trial function $\tilde{\Phi}(r)$ in both parts $\tilde{M}_I^{\{e\}}$ and $\tilde{M}_{III}^{\{e\}}$ (IV.40)-(IV.41) of the mass equivalent one has now to make use of the *general* form (III.50)-(III.51), i. e.

$$\tilde{M}_I^{\{e\}}c^2 \Rightarrow \tilde{M}_I^{\{e\}}c^2 = -\left(\frac{\pi}{2}\right)^2 \hbar c \int dr r^{\{p\}} A_I(r) \cdot \Phi_*^2 r^{2\nu} e^{-2\beta r} \quad (\text{C.7a})$$

$$\tilde{M}_{III}^{\{e\}}c^2 \Rightarrow \tilde{M}_{III}^{\{e\}}c^2 = -\left(\frac{3\pi}{8}\right)^2 \hbar c \int dr r^{\{p\}} A_{III}(r) \cdot \Phi_*^2 r^{2\nu} e^{-2\beta r}, \quad (\text{C.7b})$$

where the radial auxiliary potentials $\{p\}A_I(r)$ and $\{p\}A_{III}(r)$ are specified for general ν (in dimensionless form) by equations (B.5)-(B.6) of **App. B**. Thus one finds by explicitly carrying out the required integrations in (C.7a)-(C.7b)

$$\tilde{M}_I^{\{e\}}c^2 = -\hbar c (2\alpha_s \beta) \cdot \varepsilon_{\text{pot}}(\nu) \equiv E_I^{\{e\}} \quad (\text{C.8a})$$

$$\tilde{M}_{III}^{\{e\}}c^2 = -\hbar c (2\alpha_s \beta) \mu_R^{\{e\}}(\nu) \quad (\text{C.8b})$$

$$\mu_R^{\{e\}}(\nu) \doteq \frac{3}{128} \cdot \frac{1}{2^{4\nu}} \cdot \frac{\Gamma(4\nu + 3)}{\Gamma(2\nu + 2)^2}. \quad (\text{C.8c})$$

Clearly for $\nu = 0$, this result leads us back to the previous groundstate results (IV.40)-(IV.41). But even for $\nu \neq 0$, the present results display a structure very similar to the former groundstate situation (IV.42). Namely, the striking feature concerns here the Poisson constraint term $\tilde{N}_G^{\{e\}}$ (IV.38) which for the present situation of the excited states adopts the following form:

$$\tilde{N}_G^{\{e\}} = E_{II}^{\{e\}} + E_{III}^{\{e\}} - \tilde{M}_{III}^{\{e\}}c^2 = -\hbar c (2\alpha_s \beta) \cdot \varepsilon_G^{\{e\}} \quad (\text{C.9})$$

with

$$\varepsilon_G^{\{e\}}(\nu) \doteq {}^{(II)}\varepsilon_{\text{pot}}(\nu) + {}^{(III)}\varepsilon_{\text{pot}}(\nu) - \mu_R^{\{e\}}(\nu). \quad (\text{C.10})$$

This similarity comes about through the present identity relation (C.4a) for the potential functions $\varepsilon_{\text{pot}}(\nu)$ and ${}^{(I)}\varepsilon_{\text{pot}}(\nu)$ which entails for $\nu \neq 0$ the same equality of the energy $E_{\text{l}}^{\{e\}}$ and mass equivalent $\tilde{M}_{\text{l}}^{\{e\}}c^2$, cf. the remark above (IV.42), as is the case for the previous groundstate situation (IV.40) with $\nu = 0$. Consequently, both electrostatic contributions (C.5) and (C.9) to the energy functional (IV.29) add up in order to yield now

$$E_{\text{R}}^{\{e\}} + \lambda_{\text{G}}^{\{e\}} \cdot \tilde{N}_{\text{G}}^{\{e\}} = -\hbar c (2\alpha_s \beta) \left[\varepsilon_{\text{R}}^{\{e\}}(\nu) - 2\varepsilon_{\text{G}}(\nu) \right] = -\hbar c (2\alpha_s \beta) \cdot \varepsilon^{\{e\}}(\nu) \quad (\text{C.11a})$$

$$\varepsilon^{\{e\}}(\nu) \doteq \varepsilon_{\text{R}}^{\{e\}} - 2\varepsilon_{\text{G}}(\nu) = {}^{(I)}\varepsilon_{\text{pot}}(\nu) - {}^{(II)}\varepsilon_{\text{pot}}(\nu) - {}^{(III)}\varepsilon_{\text{pot}}(\nu) + 2\mu_{\text{R}}^{\{e\}}(\nu). \quad (\text{C.11b})$$

The crucial point with this total electrostatic contribution (C.11a) to the energy function $\tilde{E}_{\Phi}(\beta, \nu)$, to be conceived as the value of the energy functional $\tilde{E}_{[\Phi]}$ (IV.29) on the chosen trial configuration, is now that it is of the same structure as in the case for the *spherically symmetric* approximation (A.22) and for the *anisotropic* groundstate (IV.43); namely, both the gauge field energy $E_{\text{R}}^{\{e\}}$ and its mass equivalent $\tilde{M}^{\{e\}}c^2$ do contribute a linear function of the variational parameter β . On the other hand, the kinetic energy E_{kin} has been found to contribute a quadratic function of β , cf. (III.52)-(III.53); and therefore the present energy function $\tilde{E}_{\Phi}(\beta, \nu)$ for the anisotropic excited states displays again the formerly encountered shape for the isotropic situation (cf. (A.22)):

$$\tilde{E}_{\Phi}(\beta, \nu) = \frac{e^2}{a_B} \left[(2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (2a_B \beta) \cdot \varepsilon^{\{e\}}(\nu) \right], \quad (\text{C.12})$$

where merely the simple potential function $\varepsilon_{\text{pot}}(\nu)$ (A.28) is to be replaced by the present more complicated *electrostatic function* $\varepsilon^{\{e\}}(\nu)$ (C.11b). Clearly, as a consistency check one puts here $\nu = 0$ and is led back to the former groundstate result $\tilde{E}_{\Phi}(\beta)$ (IV.43).

This similarity to the former configurations of spherical symmetry (**Sect. III**) and of the anisotropic groundstate (**Subsect. IV.3**) enables us to write down immediately the result for the present anisotropic situation. The extremalization process (III.40), being exemplified for the spherically symmetric approximation through equations (A.23a)-(A.23b) in **App. A**, reduces now the two-parameter energy function $\tilde{E}_{\Phi}(\beta, \nu)$ (C.12) again

to the wanted one-parameter energy function $\mathbb{E}_*(\nu)$ (C.2). Here, the spectral function $S_\phi^{(*)}(\nu)$ is formally the same as previously for the spherically symmetric approximation, cf. (III.56a)-(III.56b), with merely the former potential function $\varepsilon_{\text{pot}}(\nu)$ being replaced now by its present “anisotropic” counterpart $\varepsilon^{\{e\}}(\nu)$ (C.11b), i. e.

$$S_\phi^{(*)}(\nu) = \frac{(\varepsilon^{\{e\}}(\nu))^2}{\varepsilon_{\text{kin}}(\nu)} . \quad (\text{C.13})$$

Consequently, the last step consists again in looking for the maximal value of $S_\phi^{(*)}(\nu)$ (\rightsquigarrow minimal value of $\mathbb{E}_*(\nu)$ (C.2)) by means of an appropriate computer program.

For our present purposes, it may be sufficient to display the result for some representative values of the variational parameter ν , see the table below. For the sake of comparison with the spherically symmetric approximation, one can introduce here the relative shift (Δ) due to the present anisotropic corrections

$$\Delta(\nu) \doteq \frac{\mathbb{E}_*(\nu) - \mathbb{E}_T(\nu)}{\mathbb{E}_T(\nu)} \equiv \frac{S_\phi(\nu) - S_\phi^{(*)}(\nu)}{S_\phi(\nu)} , \quad (\text{C.14})$$

where the energy function $\mathbb{E}_T(\nu)$ due to the spherically symmetric approximation is defined through equations (III.56a)-(III.56b). From the results of this table it becomes obvious that the anisotropy effect lifts up the energy levels of the spherically symmetric approximation, where the shift increases with increasing variational parameter ν . For instance, for $\nu = 0$, $l_\phi = 0$ one finds a shift of -0.41% (first line of the table); whereas for $\nu_* \cong 1.8$ (i. e. the first excited state) the energy shift amounts to roughly 8% which is the same deviation as is found for the difference between the spherically symmetric approximation and the conventional result (see the second line of table 1 on p. 44). However, the unacceptable feature of this result is the fact that for the excited states ($\nu > 0$) the energy levels of the spherically symmetric approximation become *lifted* instead of *lowered*, as required by the principle of minimal energy! Therefore the present anisotropy expansion (IV.9) must be replaced by a more systematic procedure (\rightsquigarrow **Sect. V**).

ν	l_φ	$S_\varphi(\nu)$ (III.56b)	$S_\varphi^{(*)}(\nu)$ (C.13)	$\Delta(\nu)$ (C.14) [%]
0	0	1.0000	1.0041...	-0.41
	1	-	-	-
$\frac{1}{2}$	0	0.7812...	0.7715...	1.24
	1	0.1562...	0.1543...	1.22
1	0	0.6302...	0.6089...	3.38
	1	0.2100...	0.2029...	3.38
$\frac{3}{2}$	0	0.5278...	0.4969...	5.85
	1	0.2262...	0.2129...	5.88
2	0	0.4546...	0.4153...	8.64
	1	0.2273...	0.2076...	8.67

Appendix D:

Exact Solutions of the Quadrupole Equation (V.34)

For the construction of solutions $\{^p\}A^{III}(r)$ to the equation (V.34) it is very convenient to pass over again to dimensionless objects, i. e. we first define the dimensionless version of $\{^p\}A^{III}(r)$ through

$$\mathcal{A}_\nu^{III}(y) \doteq (2\beta\alpha_s)^{-1} \{^p\}A^{III}(r), \quad (\text{D.1})$$

so that the quadrupole equation (V.34) reappears in the following form:

$$\left(\Delta_y - \frac{6}{y^2} \right) \mathcal{A}_\nu^{III}(y) = -\frac{10}{\pi} \frac{y^{2\nu-1} \cdot e^{-y}}{\Gamma(2\nu+2)} \quad (\text{D.2})$$

$$(y \doteq 2\beta r).$$

A first integral of this equation can easily be found here by observing that the (ordinary!) differential equation (D.2) may be rewritten in the following form

$$\frac{1}{y^4} \frac{d}{dy} \left[y^6 \cdot \frac{d}{dy} \left(\frac{\mathcal{A}_\nu^{III}(y)}{y^2} \right) \right] = -\frac{10}{\pi} \frac{y^{2\nu-1} \cdot e^{-y}}{(2\nu+1)!}, \quad (\text{D.3})$$

where, for the present purposes, we restrict ourselves to integer values of 2ν (i. e. $2\nu = 1, 2, 3, 4, \dots$). By a first integration step in (D.3) one easily arrives at the intermediate result (for $\nu \geq 1$)

$$\frac{d}{dy} \left(\frac{\mathcal{A}_\nu^{III}(y)}{y^2} \right) = -\frac{10}{\pi} (2\nu+3)(2\nu+2) \frac{1 - e^{-y} \sum_{n=0}^{2\nu+3} \frac{y^n}{n!}}{y^6}, \quad (\text{D.4})$$

which can be directly checked by means of a simple differentiation process. For the next integration step it is very advantageous to first consider the special value $\nu = 1$ for the variational parameter. In this case, one obtains from the intermediate result (D.4)

$$\mathcal{A}_1^{III}(y) = \frac{40}{\pi} \frac{1 - e^{-y} \sum_{n=0}^4 \frac{y^n}{n!}}{y^3}. \quad (\text{D.5})$$

This result for $\nu = 1$ may now be used in order to further integrate in equation (D.4) which yields for integer 2ν

$$\mathcal{A}_\nu^{\text{III}}(y) = \frac{(2\nu+3)(2\nu+2)}{20} \mathcal{A}_1^{\text{III}}(y) - \frac{10}{\pi} (2\nu+3)(2\nu+2) y^2 \cdot \sum_{n=6}^{2\nu+3} \frac{1}{n!} \int_y^\infty dy' y'^{n-6} e^{-y'} \quad (\nu \geq 1) \quad (\text{D.6})$$

(for $\nu = 1$, the second term is to be omitted). As a check, one lets act the differential operator $(\Delta_y - \frac{6}{y^2})$ upon the result in order to find that the differential equation (D.2) is actually satisfied. In the last step, one explicitly calculates the residual integral on the right-hand side of equation (D.6) and thus obtains the final result (for $\nu \geq \frac{3}{2}$)

$$\mathcal{A}_\nu^{\text{III}}(y) = \frac{(2\nu+3)(2\nu+2)}{20} \mathcal{A}_1^{\text{III}}(y) - \frac{10}{\pi} (2\nu+3)(2\nu+2) y^2 e^{-y} \sum_{n=6}^{2\nu+3} \frac{1}{n!} \sum_{m=0}^{n-6} \frac{d^m}{dy^m} (y^{n-6}) \quad (\text{D.7})$$

(for $\nu = 1$, the second term is to be omitted).

From this result it is clearly seen that the behaviour of the first anisotropic correction $\mathcal{A}_\nu^{\text{III}}(y)$ is determined by $\mathcal{A}_1^{\text{III}}(y)$ (D.5) in both the asymptotic region ($y \rightarrow \infty$) and around the origin ($y \rightarrow 0$). Since $\mathcal{A}_1^{\text{III}}(y)$ (D.5) behaves as follows

$$\lim_{y \rightarrow \infty} \mathcal{A}_1^{\text{III}}(y) \simeq \frac{40}{\pi} \cdot \frac{1}{y^3}, \quad (\text{D.8})$$

one obtains for the general $\mathcal{A}_\nu^{\text{III}}(y)$ (D.7)

$$\lim_{y \rightarrow \infty} \mathcal{A}_\nu^{\text{III}}(y) \simeq \frac{2}{\pi} (2\nu+3)(2\nu+2) \cdot \frac{1}{y^3} \quad (\text{D.9})$$

which is nothing else than the claim (V.36) at the end of **Sect.V.3**, rewritten in dimensionless form.

In order to gain some insight into the properties of the anisotropy corrections $\mathcal{A}_\nu^{\text{III}}(y)$ in the vicinity of the origin ($y = 0$), one writes down explicitly some of the lowest-order

cases:

$$\mathcal{A}_1^{\text{III}}(y) = \frac{40}{\pi} e^{-y} \sum_{n=5}^{\infty} \frac{y^{n-3}}{n!} \cong \frac{1}{3\pi} \left(y^2 - \frac{5}{6} y^3 + \frac{5}{14} y^4 - \frac{5}{48} y^5 + \dots \right) \quad (\text{D.10a})$$

$$\mathcal{A}_{\frac{3}{2}}^{\text{III}}(y) = \frac{3}{2} \mathcal{A}_1^{\text{III}}(y) - \frac{5}{12\pi} y^2 e^{-y} \cong \frac{1}{12\pi} \left(y^2 - \frac{5}{14} y^4 + \dots \right) \quad (\text{D.10b})$$

$$\mathcal{A}_2^{\text{III}}(y) = \frac{21}{10} \mathcal{A}_1^{\text{III}}(y) - \frac{1}{12\pi} e^{-y} (8y^2 + y^3) \cong \frac{1}{30\pi} \left(y^2 - \frac{5}{48} y^5 + \dots \right). \quad (\text{D.10c})$$

Observe here that with increasing ν ($\rightarrow 1, \frac{3}{2}, 2, \dots$) the anisotropic correction $\mathcal{A}_\nu^{\text{III}}(y)$ becomes smaller and smaller in the vicinity of the origin ($y \rightarrow 0$), whereas at infinity ($y \rightarrow \infty$) the correction $\mathcal{A}_\nu^{\text{III}}(y)$ becomes larger and larger, cf. (D.9). For a sketch of the three lowest-order corrections (D.10a)-(D.10c) see **Fig. D.I** below.

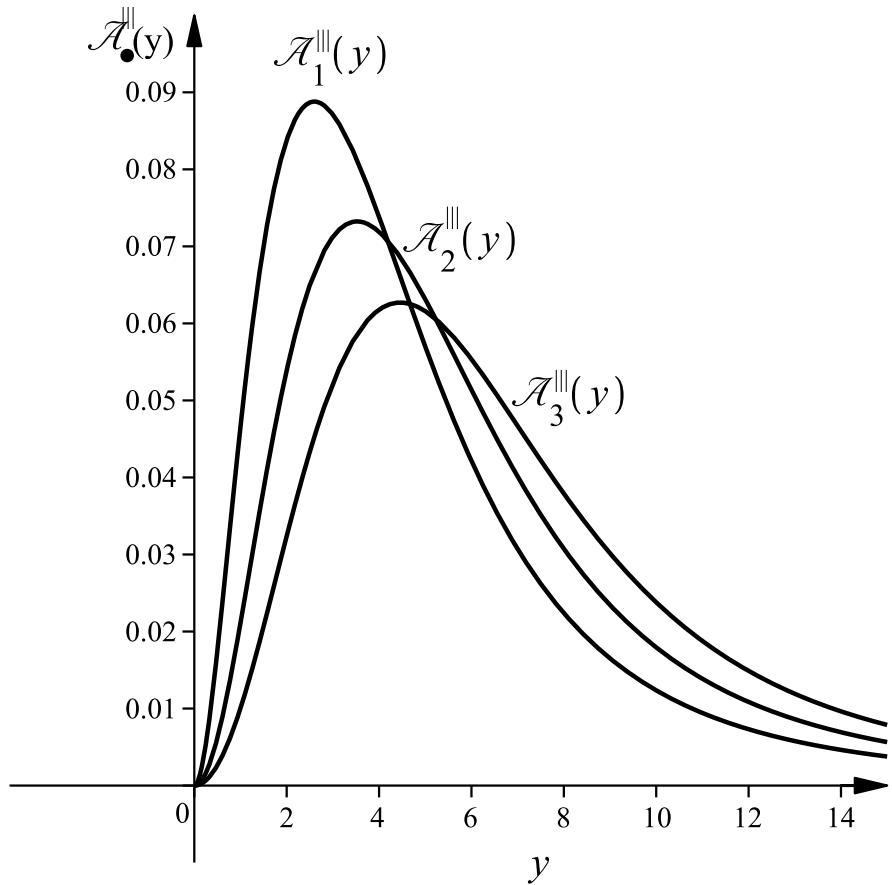


Fig. D.I Anisotropy Corrections $\mathcal{A}_\nu^{\parallel\parallel}(y)$ (D.6) The exact solution $\mathcal{A}_\nu^{\parallel\parallel}(y)$ (D.6) of the quadrupole equation (D.2) behaves like y^{-3} in the asymptotic region ($y \rightarrow \infty$), cf. (V.36); whereas in the vicinity of the origin ($y \rightarrow 0$), the behaviour is for all ν like y^2 , cf. (D.10a)-(D.10b). The magnitude of this quadrupole correction $\mathcal{A}_\nu^{\parallel\parallel}(y)$ ($\leq 1/10$) is relatively small in comparison to the magnitude of the spherically symmetric approximation $\tilde{a}_\nu(y)$, cf. (A.10), so that the anisotropy approximation can indeed be treated as a perturbation of the spherical symmetry, see the table of relative deviations $\Delta_{\{\nu\}}$ in **App. F**.

Appendix E:

Electrostatic Energy $E_R^{\{e\}}$ of the Anisotropic Configurations

Since exact solutions of the “quadrupole” equation (V.34) are at hand (see **App. D**), one can use them in order to calculate both the anisotropy energy $E_{\text{an}}^{\{e\}}$ (V.30) and its mass equivalent $\tilde{M}_{\text{an}}^{\{e\}}c^2$ (V.31) which of course must be numerically identical. This identity is itself a helpful mutual check for the numerical correctness of the electrostatic field energy and its mass equivalent. Subsequently, we will present the results for some (half-)integer values of the variational parameter ν which in **Sect. V** are then used in order to build up the “anisotropic” energy function $\mathbb{E}^{\{\text{IV}\}}(\beta, \nu)$ for the excited states, i. e. the anisotropic generalization of the “isotropic” $\mathbb{E}^{[\text{IV}]}(\beta, \nu)$ (III.55).

First, it is very convenient to introduce here again the dimensionless objects, i. e. the anisotropy energy $E_{\text{an}}^{\{e\}}$ (V.30) reads in terms of the dimensionless potential correction $\mathcal{A}_\nu^{\text{III}}(y)$ (D.1)

$$E_{\text{an}}^{\{e\}} = -\frac{\pi^2}{160}(e^2\beta) \cdot \left\{ \int_0^\infty dy y^2 \left(\frac{d\mathcal{A}_\nu^{\text{III}}}{dy} \right)^2 + 6 \int_0^\infty dy (\mathcal{A}_\nu^{\text{III}})^2 \right\} \doteq -e^2\beta \cdot \varepsilon_{\text{an}}^{\{e\}} . \quad (\text{E.1})$$

Similarly, the corresponding mass equivalent $\tilde{M}_{\text{an}}^{\{e\}}c^2$ (V.31) also reappears in terms of that dimensionless $\mathcal{A}_\nu^{\text{III}}(y)$ as follows:

$$\tilde{M}_{\text{an}}^{\{e\}}c^2 = -\frac{\pi}{16} \frac{e^2\beta}{(2\nu+1)!} \int_0^\infty dy y^{2\nu+1} e^{-y} \cdot \mathcal{A}_\nu^{\text{III}}(y) . \quad (\text{E.2})$$

The vanishing of the “anisotropic” Poisson identity $\tilde{N}_{\text{an}}^{\{e\}}$ (V.26) says now that both right-hand sides of equations (E.1) and (E.2) must be numerically identical! The subsequent table at the end of this appendix displays the results in units of $(e^2\beta)$ for some values of the variational parameter ν .

Now in order to deduce a practicable recipe for calculating the anisotropy energy $E_{\text{an}}^{\{e\}}$ (E.1) and its mass equivalent $\tilde{M}_{\text{an}}^{\{e\}}c^2$ (E.2) it is very convenient to refer the *general* case

(for integer values of 2ν) to the *special* case for $\nu = 1$, quite similarly as it has been done for the calculation of the anisotropy corrections $\mathcal{A}_\nu^{\text{III}}(y)$, see equation (D.7) of **App. D**. First, one recasts that equation (D.7) to a somewhat more concise form, i. e. we put

$$\mathcal{A}_\nu^{\text{III}}(y) = (2\nu + 3)(2\nu + 2) \cdot \left\{ \frac{\mathcal{A}_1^{\text{III}}(y)}{20} - \frac{10}{\pi} \mathcal{B}_\nu^{\text{III}}(y) \right\} , \quad (\text{E.3})$$

with the short-range constituent $\mathcal{B}_\nu^{\text{III}}(y)$ being defined through

$$\mathcal{B}_\nu^{\text{III}}(y) \doteq y^2 e^{-y} \cdot \sum_{n=6}^{2\nu+3} \frac{1}{n!} \sum_{m=0}^{n-6} \frac{d^m}{dy^m} (y^{n-6}) , \quad (\text{E.4})$$

and obeying the following differential equation

$$\begin{aligned} \left(\Delta_y - \frac{6}{y^2} \right) \mathcal{B}_\nu^{\text{III}}(y) &= \frac{y^{2\nu-1} e^{-y}}{(2\nu+3)!} - \frac{y e^{-y}}{5!} \\ (\leadsto \mathcal{B}_\nu^{\text{III}}(y) &= 0 \text{ for } \nu = 1) . \end{aligned} \quad (\text{E.5})$$

Next, one could substitute this new form $\mathcal{A}_\nu^{\text{III}}(y)$ (E.3) into the equation (E.1) and would then find the desired anisotropy correction $E_{\text{an}}^{\{\text{e}\}}$ being expressed in terms of $\mathcal{A}_1^{\text{III}}(y)$ and $\mathcal{B}_\nu^{\text{III}}(y)$. We do not present here that equation, but rather prefer to calculate the corresponding mass equivalent $\tilde{\mathbb{M}}_{\text{an}}^{\{\text{e}\}} c^2$ (E.2), namely on behalf of its more convenient handling. Indeed, if we introduce two auxiliary objects \mathbb{K}_ν and \mathbb{L}_ν through

$$\mathbb{K}_\nu \doteq \int_0^\infty dy y^{2\nu+1} e^{-y} \cdot \mathcal{B}_\nu^{\text{III}}(y) \quad (\text{E.6a})$$

$$\mathbb{L}_\nu \doteq \frac{\pi}{40} \frac{1}{(2\nu-2)!} \int_0^\infty dy y^{2\nu+1} e^{-y} \cdot \mathcal{A}_1^{\text{III}}(y) , \quad (\text{E.6b})$$

then the mass equivalent $\tilde{\mathbb{M}}_{\text{an}}^{\{\text{e}\}} c^2$ (E.2) reads in terms of these newly introduced objects

$$\begin{aligned} \tilde{\mathbb{M}}_{\text{an}}^{\{\text{e}\}} c^2 &= -e^2 \beta \cdot \frac{(2\nu+3)(2\nu+2)}{(2\nu+1)!} \left\{ \frac{(2\nu-2)!}{8} \cdot \mathbb{L}_\nu - \frac{5}{8} \cdot \mathbb{K}_\nu \right\} \\ &\doteq -e^2 \beta \cdot \mu_{\text{an}}^{\{\text{e}\}}(\nu) . \end{aligned} \quad (\text{E.7})$$

The straightforward integration yields

$$\mathbb{K}_\nu = \sum_{n=0}^{2\nu-3} \frac{n!}{(n+6)!} \sum_{m=0}^n \frac{1}{2^{2\nu+4+n-m}} \cdot \frac{(2\nu+3+n-m)!}{(n-m)!} \quad (\text{E.8a})$$

$$\mathbb{L}_\nu = 1 - \sum_{n=0}^4 \frac{1}{n! 2^{2\nu-1+n}} \cdot \frac{(2\nu-2+n)!}{(2\nu-2)!}. \quad (\text{E.8b})$$

The subsequent table presents the value of the “anisotropic” mass equivalent $\tilde{\mathbb{M}}_{\text{an}}^{\{e\}} c^2$ (E.7) for some representative values of the variational parameter ν . Since the “anisotropic” Poisson identity $\tilde{\mathbb{N}}_{\text{an}}^{\{e\}}$ vanishes for our exact solution $\mathcal{A}_\nu^{\text{III}}(y)$ (E.3)-(E.4) of the (dimensionless) quadrupole equation (D.3), this table simultaneously displays the “anisotropic” gauge field energy $E_{\text{an}}^{\{e\}}$ (E.1) for those specified values of ν . This then admits to determine also the total gauge field energy $E_{\text{R}}^{\{e\}}$ (V.21) as the sum of its “isotropic” part $E_{\text{R}}^{\{e\}}$ (V.15) and its “anisotropic” counterpart $E_{\text{an}}^{\{e\}}$ (E.1):

$$E_{\text{R}}^{\{e\}} = E_{\text{R}}^{\{e\}} + E_{\text{an}}^{\{e\}} = -(e^2 \beta) \{ 2\varepsilon_{\text{pot}}(\nu) + \mu_{\text{an}}^{\{e\}}(\nu) \} = -e^2 \beta \cdot 2\varepsilon_{\text{tot}}^{\{e\}}(\nu) \quad (\text{E.9a})$$

$$\varepsilon_{\text{tot}}^{\{e\}}(\nu) \doteq \varepsilon_{\text{pot}}(\nu) + \frac{1}{2} \mu_{\text{an}}^{\{e\}}(\nu). \quad (\text{E.9b})$$

In order to better estimate the magnitude of the anisotropy corrections, it is useful to introduce the relative magnitude $\Delta_{\text{an}}^{\{e\}}(\nu)$ through

$$\Delta_{\text{an}}^{\{e\}}(\nu) \doteq \frac{E_{\text{an}}^{\{e\}}}{E_{\text{R}}^{\{e\}}} = \frac{\mu_{\text{an}}^{\{e\}}(\nu)}{2\varepsilon_{\text{tot}}^{\{e\}}(\nu)} = \frac{\mu_{\text{an}}^{\{e\}}(\nu)}{2\varepsilon_{\text{pot}}(\nu) + \mu_{\text{an}}^{\{e\}}(\nu)}. \quad (\text{E.10})$$

ν	\mathbb{K}_ν (E.8a)	\mathbb{L}_ν (E.8b)	$\mu_{\text{an}}^{\{e\}}(\nu)$ (E.7)	$2 \cdot \varepsilon_{\text{pot}}(\nu)$ (A.28)	$2 \cdot \varepsilon_{\text{tot}}^{\{e\}}(\nu)$ (E.9b)	$\Delta_{\text{an}}^{\{e\}}(\nu) [\%]$ (E.10)
1		$\frac{1}{32}$ $= 3.125 \cdot 10^{-2}$	$\frac{5}{384}$ $\simeq 1.3020 \cdot 10^{-2}$	$\frac{11}{24}$ $\simeq 4.5833 \cdot 10^{-1}$	$\frac{181}{384}$ $\simeq 4.7135 \cdot 10^{-1}$	2.76
$\frac{3}{2}$	$\frac{1}{128}$ $\simeq 7.8125 \cdot 10^{-4}$	$\frac{7}{64}$ $= 1.09375 \cdot 10^{-1}$	$\frac{45}{4096}$ $\simeq 1.09863 \cdot 10^{-2}$	$\frac{93}{256}$ $\simeq 3.6328 \cdot 10^{-1}$	$\frac{1533}{4096}$ $\simeq 3.7426 \cdot 10^{-1}$	2.93
2	$\frac{3}{64}$ $\simeq 4.6875 \cdot 10^{-2}$	$\frac{29}{128}$ $\simeq 2.2656 \cdot 10^{-1}$	$\frac{49}{5120}$ $\simeq 9.5703 \cdot 10^{-3}$	$\frac{193}{640}$ $\simeq 3.0156 \cdot 10^{-1}$	$\frac{1593}{5120}$ $\simeq 3.1113 \cdot 10^{-1}$	3.07
$\frac{5}{2}$	$\frac{267}{1024}$ $\simeq 2.6074 \cdot 10^{-1}$	$\frac{93}{256}$ $\simeq 3.6325 \cdot 10^{-1}$	$\frac{2093}{245760}$ $\simeq 8.5164 \cdot 10^{-3}$	$\frac{793}{3072}$ $\simeq 2.58138 \cdot 10^{-1}$	$\frac{65533}{245760}$ $\simeq 2.66654 \cdot 10^{-1}$	3.19
3	$\frac{1575}{1024}$ $\simeq 1.53808$	$\frac{1}{2}$ $= 0.5$	$\frac{4413}{573440}$ $\simeq 7.6956 \cdot 10^{-3}$	$\frac{1619}{7168}$ $\simeq 2.25864 \cdot 10^{-1}$	$\frac{133933}{573440}$ $\simeq 2.3356 \cdot 10^{-1}$	3.29
4	7.0229e+01	7.2559e-01	6.4899e-03	1.8101e-01	1.8750e-01	3.46
5	4.6795e+03	8.6658e-01	5.6388e-03	1.5124e-01	1.5688e-01	3.59
6	4.4549e+05	9.4077e-01	5.0013e-03	1.3000e-01	1.3500e-01	3.70
7	5.8810e+07	9.7548e-01	4.5034e-03	1.1407e-01	1.1857e-01	3.80
8	1.0442e+10	9.9039e-01	4.1024e-03	1.0167e-01	1.0577e-01	3.88
9	2.4216e+12	9.9640e-01	3.7717e-03	9.1728e-02	9.5500e-02	3.95
10	7.1438e+14	9.9870e-01	3.4938e-03	8.3582e-02	8.7076e-02	4.01
20	4.3817e+43	1.0000e+00	2.0511e-03	4.4495e-02	4.6547e-02	4.41
30	1.6409e+77	1.0000e+00	1.4718e-03	3.0423e-02	3.1895e-02	4.61
40	6.9176e+113	1.0000e+00	1.1543e-03	2.3146e-02	2.4300e-02	4.75
50	5.1832e+152	1.0000e+00	9.5231e-04	1.8692e-02	1.9644e-02	4.85
60	2.3612e+193	1.0000e+00	8.1198e-04	1.5682e-02	1.6494e-02	4.92
70	3.2381e+235	1.0000e+00	7.0856e-04	1.3511e-02	1.4220e-02	4.98
80	8.1332e+278	1.0000e+00	6.2905e-04	1.1870e-02	1.2499e-02	5.03
90	2.5844e+323	1.0000e+00	5.6593e-04	1.0587e-02	1.1153e-02	5.07
100	7.8031e+368	1.0000e+00	5.1458e-04	9.5545e-03	1.0069e-02	5.11

It is instructive to see from this table that the anisotropy correction in the vicinity of the first excited state $n_\varphi = 2$ (which has $\nu_* \simeq 1.8$, see **table 1** on p. 44) lowers the electrostatic interaction energy $E_R^{[e]}$ of the spherically symmetric approximation by some 3%. The smallness of this anisotropy effect is the reason why the spherically symmetric approximation produces preliminary predictions with acceptable exactness, i. e. roughly 8% deviation for the first excited state $n_\varphi = 2$ (second line of **table 1** on p. 44). Observe, however, that the present anisotropy corrections ($\simeq 3\%$) must improve the RST predictions for the binding energy by a factor of two (i. e. roughly 6%) because the total binding energy \mathbb{E}_T amounts to only half the value of the interaction energy $E_R^{[e]}$. For this reason, the deviation of the RST prediction for the first excited state ($n_\varphi = 2$) becomes reduced from 8.8% (**table 1**) to 3% (see **App. F**).

Appendix F:

Extremalization Process (V.38a)-(V.38b) for the Anisotropic Configurations

If all constraints are duly regarded, the original energy functional $\tilde{\mathbb{E}}_{[T]}$ ultimately consists of two terms only, cf. (V.37), i. e. the kinetic energy E_{kin} (III.52)-(III.53) and the gauge field energy $E_R^{\{e\}}$ (V.21) which is the sum of the “isotropic” part $E_R^{[e]}$ (V.14) and the “anisotropic” part $E_{\text{an}}^{\{e\}}$ (V.30). From the principal point of view, both kinds of energy E_{kin} and $E_R^{\{e\}}$ are of equivalent conceptual importance; but from a more technical viewpoint the gauge field part $E_R^{\{e\}}$ (and especially its anisotropic constituent $E_{\text{an}}^{\{e\}}$ (V.30)) requires greater effort for its exact calculation (for general ν). Therefore we are satisfied for the moment with specifying $E_{\text{an}}^{\{e\}}$ for integer 2ν only, see **App. E**. But this then implies that also the total energy function $\mathbb{E}^{\{IV\}}(\beta, \nu)$ (V.39) and its reduced form $\mathbb{E}_{\{\nu\}}$ (V.40) can be specified only for integer values of 2ν . On the other hand, for the extremalization procedure (III.40), as being specified by equations (V.38a)-(V.38b), we need a continuously differentiable energy function $\mathbb{E}_{\{\nu\}}$ whose stationary points ($\frac{d\mathbb{E}_{\{\nu\}}}{d\nu} = 0$) determine the wanted energy spectrum. Therefore, as an auxiliary construction, we are satisfied for the present purposes with a supporting polynomial (of appropriate rank) which has in common with the spectral function $S_\phi^{\{a\}}(\nu)$ (V.42) its values on some suitable integers 2ν . The extremalization process ($\frac{dS_\phi^{\{a\}}(\nu)}{d\nu} = 0$) is then carried through with the help of this supporting polynomial.

For given quantum number l_ϕ ($= 0, 1, 2, 3, \dots$) of angular momentum it will not be necessary to take into account the values of $S_\phi^{\{a\}}(\nu)$ on all integers 2ν but one merely considers a limited number of supporting points (6, say) around the expected stationary point of $S_\phi^{\{a\}}(\nu)$. For an estimate of the latter stationary point one may resort to **table 1** (p. 44) because the anisotropy correction will be sufficiently small so that the stationary points due to the spherically symmetric approximation will not be shifted too far away.

Finally, it may also be interesting to see the extent to which the “isotropic” energy curve $\mathbb{E}_T(\nu)$ (III.56a)-(III.56b) becomes lowered to the “anisotropic” $\mathbb{E}_{\{\nu\}}^\phi$ (V.41) as consequence of the anisotropy effect. To this end, one defines the corresponding relative energy shift $\Delta_{\{\nu\}}$ through

$$\begin{aligned}\Delta_{\{\nu\}} &\doteq \frac{\mathbb{E}_{\{\nu\}}^\phi - \mathbb{E}_T(\nu)}{|\mathbb{E}_T(\nu)|} = \frac{S_\phi(\nu) - S_\phi^{\{a\}}(\nu)}{S_\phi(\nu)} \\ &= \frac{\varepsilon_{\text{pot}}^2(\nu) - \varepsilon_{\text{tot}}^{\{e\}}(\nu)^2}{\varepsilon_{\text{pot}}^2(\nu)} = 1 - \left(\frac{\varepsilon_{\text{tot}}^{\{e\}}(\nu)}{\varepsilon_{\text{pot}}(\nu)} \right)^2,\end{aligned}\quad (\text{F.1})$$

see the table below.

Perhaps it is instructive to exemplify the proposed extremalization process by considering in some detail the first excited state $n_\phi = 2$ ($\rightsquigarrow l_\phi = 1$). In order to write down the values of the spectral function $S_\phi^{\{a\}}(\nu)$ (V.42) on the integers 2ν , one takes over the potential function $\varepsilon_{\text{tot}}^{\{e\}}(\nu)$ from equations (E.9a)-(E.9b) of **App. E** in combination with (E.7), whereas the kinetic function $\varepsilon_{\text{kin}}(\nu)$ has already been specified by equation (III.53). In this way, one sets up the subsequent table for the values of the spectral function $S_\phi^{\{a\}}(\nu)$ (on the integers of 2ν) in the vicinity of its extremal value $\nu_*^{[2]}$ ($\nu_*^{[2]} \simeq 1.7942$ for the first excited state ($n_\phi = 2$) in the spherically symmetric approximation, see **table 1** on p. 44). For an evaluation of the present RST results recall also the conventional prediction (I.4), which for the value of the spectral function due to the first excited state ($n_c = 2$) would yield $(\frac{1}{2})^2 = 0.25$. (Compare this to the subsequent values of $S_\phi^{\{a\}}(\nu)$ for $\nu = \frac{3}{2}$ and $\nu = 2$)

ν	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3
$S_\phi^{\{a\}}(\nu)$ (V.41)	$\left(\frac{181}{384}\right)^2$ $\simeq 0.22217$	$\frac{12}{7} \cdot \left(\frac{1533}{4096}\right)^2$ $\simeq 0.24013$	$10 \cdot \left(\frac{1593}{10240}\right)^2$ $\simeq 0.24200$	$\frac{10}{3} \cdot \left(\frac{65533}{245760}\right)^2$ $\simeq 0.23701$	$\frac{84}{5} \cdot \left(\frac{133933}{1146880}\right)^2$ $\simeq 0.22911$
$\Delta_{\{\nu\}}$ (F.1)	-5.76%	-6.13%	-6.44%	-6.70%	-6.93%

It is clearly seen from this table that the “isotropic” energy curve $\mathbb{E}_T(\nu)$ (III.56a)-(III.56b) becomes *lowered* in the vicinity of the first excited state (which has $\nu_*^{[2]} \simeq 1.79$)

by roughly 6%; and this evidently yields an important improvement of the 8.8% deviation of the spherically symmetric approximation from the conventional results (\sim 2nd line of the **table 1** on p. 44). Recall here also the failure of the former series expansion (IV.9) of the gauge potential $\{^p\}A_0(r, \vartheta)$ as it is expressed by the table in **App. C**. Indeed, in place of the unrealistic *raising* of the energy curve by 8% we observe now a *lowering* by some 6%!

For exemplifying our approximative method of determining the binding energy for the selected quantum number $n_\varphi = 2$, we construct the supporting polynomial $S_2(\nu)$ as

$$\begin{aligned} S_2(\nu) = & -0.000000111342528740459 \cdot \nu^{10} + 0.00000441158546612208 \cdot \nu^9 \\ & - 0.0000783955928235642 \cdot \nu^8 + 0.000825779502976810 \cdot \nu^7 \\ & - 0.00574182989858913 \cdot \nu^6 + 0.0277779729669865 \cdot \nu^5 - 0.0959826304956328 \cdot \nu^4 \\ & + 0.238726544780364 \cdot \nu^3 - 0.419428837290107 \cdot \nu^2 + 0.460369057103840 \cdot \nu \\ & + 0.015702789114075 \end{aligned} \tag{F.2}$$

which can easily be checked to agree with $S_2^{\{a\}}(\nu)$ (V.42) on the values $\nu = 1, \frac{3}{2}, 2, \frac{5}{2}, 3$ (see the above table for $S_\varphi^{\{a\}}(\nu)$ with the deviation $\Delta\{\nu\}$). Next, the maximal value of $S_2(\nu)$ (F.2) is found as

$$S_2|_{\max} = 0.2424\dots \tag{F.3}$$

at the value $\nu_*^{\{2\}}$ of the variational parameter

$$\nu_*^{\{2\}} = 1.83299\dots \tag{F.4}$$

(see the figure below). Thus the RST prediction for the energy of the first excited state ($E_\varphi^{\{2\}}$, say) is obtained as

$$E_\varphi^{\{2\}} = -\frac{e^2}{4a_B} \cdot S_2|_{\max} = -6,8029 \cdot 0.2424\dots [\text{eV}] = -1,649\dots [\text{eV}] . \tag{F.5}$$

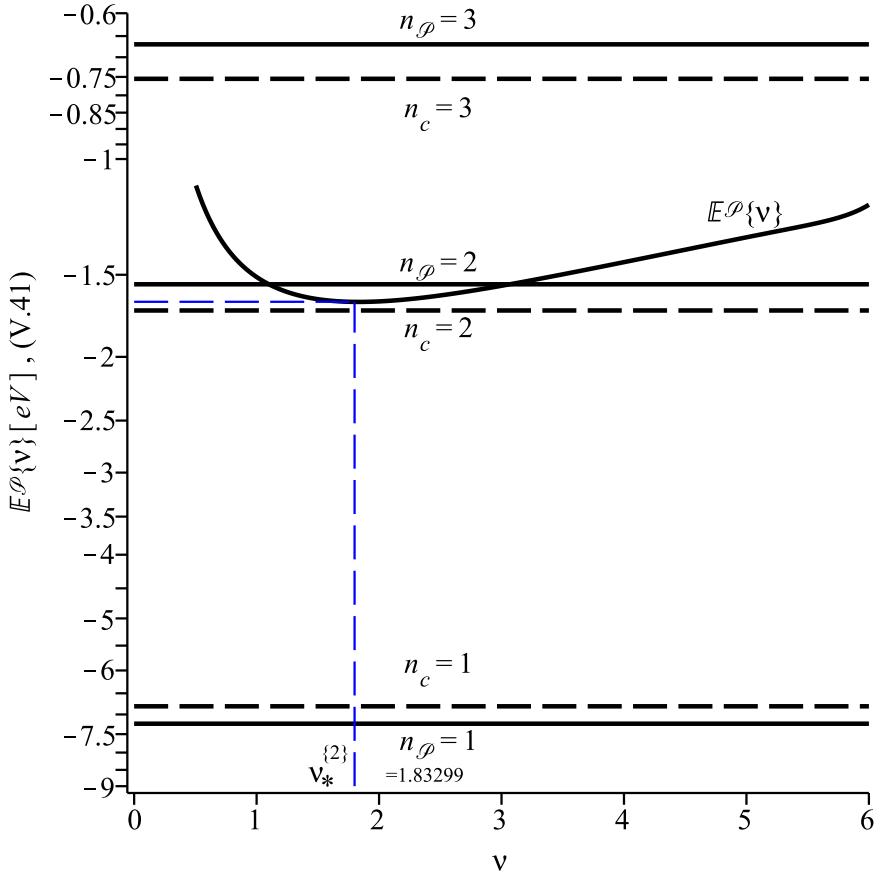


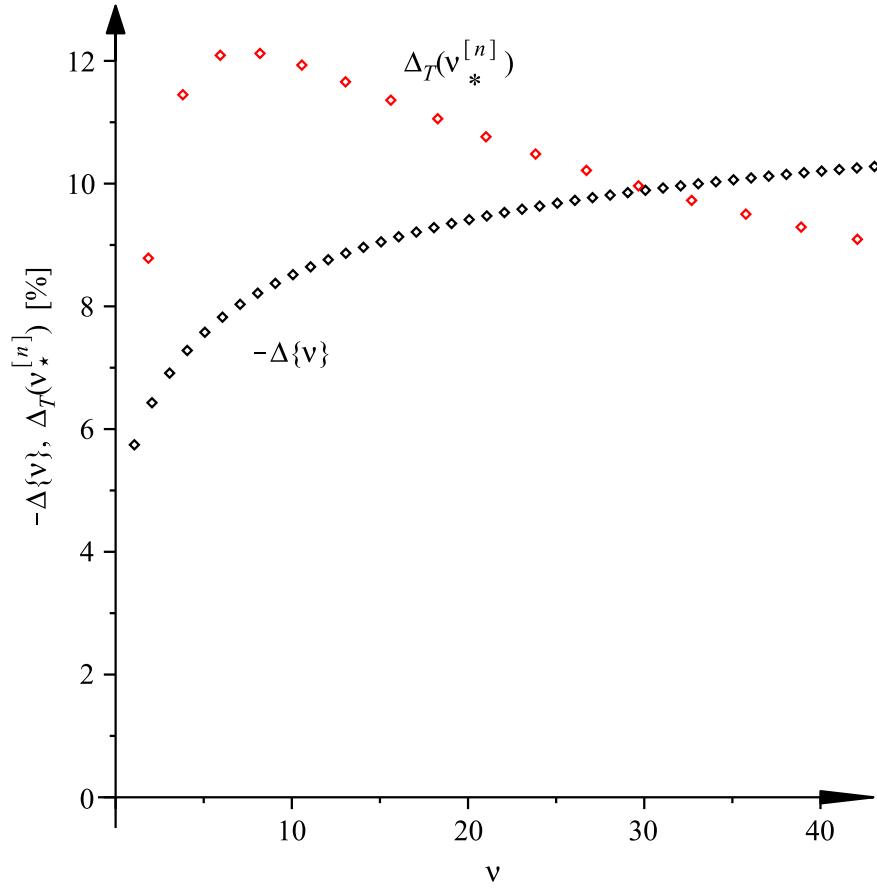
Fig. F.I *Positronium Energy and Maximal Value of the Spectral Function $S_{\phi}^{\{a\}}(\nu)$ (V.42)*

From the smallest (but integer) values of 2ν (see the table on p.114) one constructs the interpolating polynomial $S_2(\nu)$ (F.2) as an approximation to the spectral function $S_2^{\{a\}}(\nu)$ (V.42). Its maximal value (F.3) determines the energy $\mathbb{E}_{\phi}^{\{2\}}$ (F.5) of the first excited state ($n_{\phi} = 2 \leftrightarrow l_{\phi} = 1$). This “anisotropic” result deviates now from the corresponding conventional prediction (I.4) by only 3%. Thus the present anisotropic correction *improves* the “isotropic” RST prediction (solid line) from 8,8% deviation (cf. **table 1** on p. 44) to 3% deviation (with respect to the conventional prediction, broken line) which is a reduction of the deviation of roughly 66%, see also **table 2** on p. 77 for the case of higher excited states.

The 66% reduction of the deviation (from the conventional results) naturally leads us to the question of how large this decrease may be for the higher excited states ($l_\phi > 1$)? In order to get some feeling for this, one may sketch the “correction function” $\Delta\{\nu\}$ (F.1) over the variational parameter ν , see **Fig.F.II** below. Here it is satisfying to observe a decrease of deviation which ranges from 5,76% for $\nu = 1$ up to 11% for $\nu = 100$. The latter case ($\nu \simeq 100$) is due to a quantum number of $n_\phi \simeq 35$ (see table 1). It becomes obvious from this diagram that the “anisotropic” correction $\Delta\{\nu\}$ is countercurrent to the “isotropic” deviation $\Delta_T[\nu]$ due to the spherically symmetric approximation **Sect.III**, being defined through

$$\Delta_T(\nu_*^{[n]}) \doteq \frac{E_{\text{conv}}^{(n)} - E_T(\nu_*^{[n]})}{E_{\text{conv}}^{(n)}} . \quad (\text{F.6})$$

Indeed, this object quantifies the extent of deviation of our “isotropic” RST predictions from their conventional counterpart (I.4) and is displayed in the last column of **table 1** on p. 44; and when this deviation function $\Delta_T(\nu_*^{[n]})$ (F.6) is also represented in **Fig.F.II**, it becomes evident that for increasing ν it runs countercurrently to the present correction function $\Delta\{\nu\}$ (F.1). But this then entails the consequence that both curves must intersect at a certain value of ν (ν_x , say); and such an intersection means that the conventional and RST predictions will agree in the vicinity of that ν_x (see **Fig.F.II** below which yields $\nu_x \simeq 30$ corresponding to quantum number $n_\phi \simeq 15$). See also the discussion of this effect below **table 2** on p. 77.



**Fig. F.II Relative Anisotropy Correction $\Delta\{\nu\}$ (F.1)
and “Isotropic” Deviations $\Delta_T(\nu_*^{[n]})$ (F.6)**

The consideration of the anisotropy effect in the first approximation order ($\sim \{p\} A^{\parallel\parallel}(r)$) yields a relative lowering of the “isotropic” RST predictions $E_T(\nu)$ (III.56a) by $\Delta\{\nu\}$ percent, cf. (F.1). Since these “isotropic” predictions yield always higher energy than their conventional counterparts (I.4), their lowering by the anisotropy effect yields considerable improvement of the RST predictions for the low excited states (**table 2** on p. 77). But since the “anisotropic” deviation $\Delta\{\nu\}$ increases up to 11% (for $\nu \rightarrow \infty$), the decreasing “isotropic” deviation $\Delta_T(\nu_*^{[n]})$ (last column of **table 1** on p. 44) must become compensated by $\Delta\{\nu\}$ for some value ν_x of ν (here $\nu_x \simeq 30$, i.e. $n_\phi \simeq 15$); and in the vicinity of this ν_x the RST predictions will then agree with the conventional results, see the discussion below equ. (F.6) and **table 2** on p. 77.

Appendix G:

Poisson Identity and Generalized Trial Amplitude

For the numerical exploitation of the “isotropic” Poisson identity (III.47) it is very convenient to rescale again both the gauge potential ${}^{[p]}A_0(r)$ and the generalized trial amplitude $\tilde{\Phi}(r)$ (VI.1)-(VI.3b). For the latter object, one puts

$$\begin{aligned}\tilde{\Phi}_b(r) &= \sqrt{\frac{2}{\pi}} \frac{2\beta}{\sqrt{\Gamma(2\nu+2)}} \cdot \tilde{\Phi}_{\nu p}(y) \\ (y &:= 2\beta r)\end{aligned}\tag{G.1}$$

so that the dimensionless trial amplitude $\tilde{\Phi}_{\nu p}(y)$ appears in the following form

$$\tilde{\Phi}_{\nu p}(y) = y^\nu (p_0 + p_1 y) e^{-\frac{y}{2}}.\tag{G.2}$$

Next, it is necessary to look for the (exact) solution of the Poisson equation (III.36) when the trial amplitude $\tilde{\Phi}(r)$ in that equation is given by the three-parameter ansatz (VI.1)-(VI.3b), i. e. in dimensionless form (G.1)-(G.2). The corresponding Poisson equation reads explicitly

$$\begin{aligned}\frac{d^2 \tilde{a}_{\nu p}(y)}{dy^2} + \frac{2}{y} \frac{d\tilde{a}_{\nu p}(y)}{dy} &= -\frac{(p_0^2 \cdot y^{2\nu-1} + 2p_0 p_1 \cdot y^{2\nu} + p_1^2 \cdot y^{2\nu+1}) e^{-y}}{\Gamma(2\nu+2)} \\ ({}^{[p]}A_0(r) &\doteqdot 2\beta \alpha_s \tilde{a}_{\nu p}(y)).\end{aligned}\tag{G.3}$$

Obviously, the generalized potential $\tilde{a}_{\nu p}(y)$ collapses here to the former potential $\tilde{a}_\nu(y)$ (A.8) if the parameter p_1 tends to zero, because the present equation (G.3) becomes in this limit ($p_1 \rightarrow 0$) identical to the former Poisson equation (A.1) for the original ansatz (III.50)-(III.51). Indeed, the present generalized Poisson equation (G.3) is closely related to its precursor (A.1). This becomes readily more obvious by exploiting the fact that (G.3) is a linear inhomogeneous equation where the inhomogeneity is essentially a quadratic polynomial with respect to the variational parameters p_0, p_1 . For this reason,

the solution $a_{\nu p}(y)$ may be written as a superposition of three solutions $a_\nu(y)$ of the simple precursor (A.1):

$$\tilde{a}_{\nu p}(y) = -\frac{p_0^2 \cdot a_\nu(y) + 2p_0 p_1 \cdot a_{\nu+\frac{1}{2}}(y) + p_1^2 \cdot a_{\nu+1}(y)}{\Gamma(2\nu+2)}, \quad (\text{G.4})$$

where the functions $a_\nu(y)$ are (exact) solutions of the (slightly modified) precursor equation (A.1)

$$\frac{d^2 a_\nu(y)}{dy^2} + \frac{2}{y} \frac{da_\nu(y)}{dy} = y^{2\nu-1} \cdot e^{-y}. \quad (\text{G.5})$$

Quite analogously to the former situation (A.17) one introduces here the dimensionless field strength $\tilde{e}_{\nu p}(y)$ through

$$\tilde{e}_{\nu p}(y) \doteq \frac{d\tilde{a}_{\nu p}(y)}{dy} \quad (\text{G.6})$$

which then is subjected to the source equation

$$\frac{d\tilde{e}_{\nu p}(y)}{dy} + \frac{2}{y} \tilde{e}_{\nu p}(y) = -\frac{(p_0^2 \cdot y^{2\nu-1} + 2p_0 p_1 \cdot y^{2\nu} + p_1^2 \cdot y^{2\nu+1})e^{-y}}{\Gamma(2\nu+2)}. \quad (\text{G.7})$$

This is the same situation as with the Poisson equation (G.3) so that the field strength $\tilde{e}_{\nu p}(y)$ can also be written as a sum of three terms, i. e. we may put

$$\tilde{e}_{\nu p}(y) = -\frac{p_0^2 \cdot e_\nu(y) + 2p_0 p_1 \cdot e_{\nu+\frac{1}{2}}(y) + p_1^2 \cdot e_{\nu+1}(y)}{\Gamma(2\nu+2)}, \quad (\text{G.8})$$

so that the simple field strength $e_\nu(y)$ obeys the source equation

$$\frac{de_\nu(y)}{dy} + \frac{2}{y} e_\nu(y) = y^{2\nu-1} \cdot e^{-y}. \quad (\text{G.9})$$

Comparing now this source equation for the field strength $e_\nu(y)$ to the Poisson equation (G.5) for the potentials $a_\nu(y)$ one recovers the field strengths $e_\nu(y)$ as the simple derivatives of the corresponding potentials $a_\nu(y)$, i. e.

$$e_\nu(y) = \frac{da_\nu(y)}{dy}. \quad (\text{G.10})$$

Consequently, since the solutions of the Poisson equation (G.5) can easily be obtained for integer 2ν , cf. (A.7)

$$a_\nu(y) = -\frac{(2\nu+1)!}{y} \left\{ 1 - e^{-y} \cdot \sum_{n=0}^{2\nu} \frac{2\nu+1-n}{2\nu+1} \cdot \frac{y^n}{n!} \right\}, \quad (\text{G.11})$$

and the solutions of the source equation (G.9) for the field strengths $e_\nu(y)$ are obtained from this result by the simple differentiation process (G.10) as

$$e_\nu(y) = \frac{(2\nu+1)!}{y^2} \left\{ 1 - e^{-y} \cdot \sum_{n=0}^{2\nu+1} \frac{y^n}{n!} \right\}, \quad (\text{G.12})$$

cf. (A.18). Clearly, the latter two results for integer 2ν may be generalized to arbitrary real values of the variational parameter ν and do then appear in the following form:

$$a_\nu(y) = -\Gamma(2\nu+1) \cdot \left\{ 1 - e^{-y} \cdot \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu+2+n)} y^{2\nu+n} \right\} \quad (\text{G.13a})$$

$$e_\nu(y) = \Gamma(2\nu+2) e^{-y} \cdot \sum_{n=0}^{\infty} \frac{y^{2\nu+n}}{\Gamma(2\nu+3+n)}, \quad (\text{G.13b})$$

cf. (A.8) and (A.19).

But now that both the generalized potentials $\tilde{a}_{\nu p}(y)$ (G.4) and $\tilde{e}_{\nu p}(y)$ (G.8) are explicitly known, one can realize the Poisson identity (III.47) within the present framework of the generalized trial ansatz (VI.1)-(VI.2). First, consider the gauge field energy $E_R^{[e]}$ (III.45) which may be rewritten in terms of the dimensionless objects as follows

$$E_R^{[e]} = -\hbar c (2\alpha_s \beta) \int_0^\infty dy y^2 \left(\frac{d\tilde{a}_{\nu p}(y)}{dy} \right)^2 = -\hbar c (2\alpha_s \beta) \int_0^\infty dy y^2 \tilde{e}_{\nu p}^2(y). \quad (\text{G.14})$$

Inserting here the dimensionless field strengths $\tilde{e}_{\nu p}(y)$ (G.8) recasts the gauge field energy $E_R^{[e]}$ into the following shape

$$E_R^{[e]} = -\frac{e^2}{a_B} (2\beta a_B) \cdot \varepsilon_{\text{pot}}(\nu, p_0, p_1). \quad (\text{G.15})$$

This is indeed a result which looks very similar to the former case (III.54) for the simpler trial amplitude (III.50)-(III.51); but the present potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ emerges now as a polynomial of fourth order with respect to the additional parameters p_0 and p_1 , i. e.

$$\varepsilon_{\text{pot}}(\nu, p_0, p_1) = \varepsilon_{\text{pot}}(\nu) \cdot p_0^4 + 4p_0^3 p_1 \cdot \varepsilon_I(\nu) + 4p_0^2 p_1^2 \cdot \varepsilon_{II}(\nu) + 4p_0 p_1^3 \cdot \varepsilon_{III}(\nu) + p_1^4 \cdot \varepsilon_{IV}(\nu), \quad (\text{G.16})$$

with the potential functions being given by

$$\varepsilon_{\text{pot}}(\nu) = \int_0^\infty dy y^2 \left(\frac{e_\nu(y)}{\Gamma(2\nu + 2)} \right)^2 \quad (\text{G.17a})$$

$$\varepsilon_I(\nu) = \int_0^\infty dy y^2 \frac{e_\nu(y) \cdot e_{\nu+\frac{1}{2}}(y)}{\Gamma(2\nu + 2)^2} \quad (\text{G.17b})$$

$$\varepsilon_{II}(\nu) = \int_0^\infty dy y^2 \frac{e_{\nu+\frac{1}{2}}(y) \cdot e_{\nu+\frac{1}{2}}(y) + \frac{1}{2} e_\nu(y) \cdot e_{\nu+1}(y)}{\Gamma(2\nu + 2)^2} \quad (\text{G.17c})$$

$$\varepsilon_{III}(\nu) = \int_0^\infty dy y^2 \frac{e_{\nu+\frac{1}{2}}(y) \cdot e_{\nu+1}(y)}{\Gamma(2\nu + 2)^2} \quad (\text{G.17d})$$

$$\varepsilon_{IV}(\nu) = \int_0^\infty dy y^2 \left(\frac{e_{\nu+1}(y)}{\Gamma(2\nu + 2)} \right)^2. \quad (\text{G.17e})$$

Since the field strengths $e_\nu(y)$ are explicitly known, all the potential functions (G.17a)-(G.17e) can now be explicitly calculated. For the first one, i. e. (G.17a), one finds

$$\begin{aligned} \varepsilon_{\text{pot}}(\nu) &= \frac{1}{2^{4\nu+3}} \sum_{m,n=0}^{\infty} \frac{1}{2^{m+n}} \cdot \frac{\Gamma(4\nu + 3 + m + n)}{\Gamma(2\nu + 3 + m) \cdot \Gamma(2\nu + 3 + n)} \\ &\stackrel{2\nu \text{ int.}}{\Rightarrow} \sum_{\substack{m,n=0 \\ (m+n \geq 2)}}^{2\nu+1} \frac{1}{2^{m+n-1}} \cdot \frac{(m+n-2)!}{m! n!} - 2 \sum_{n=2}^{2\nu+1} \frac{(n-2)!}{n!}. \end{aligned} \quad (\text{G.18})$$

Here, the result in the first line refers to general (real) values of the variational parameter ν and the second line presents the specialization to integer values of 2ν . Clearly, this first potential function $\varepsilon_{\text{pot}}(\nu)$ (G.18) is nothing else than the corresponding result (A.28) for the simple trial function (III.50) which has $p_1 = 0$; and therefore the present generalized potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ (G.16) must of course collapse to $\varepsilon_{\text{pot}}(\nu)$ (A.28) for $p_1 \rightarrow 0$.

But for non-vanishing variational parameter p_1 , the other potential functions $\varepsilon_I, \dots, \varepsilon_{IV}$ (G.17b)-(G.17e) yield important contributions and must be explicitly known for the extremalization process (III.40) due to the *principle of minimal energy* (the role played by the third variational parameter ν_2 is played here by the parameter p_1 , cf. (VI.1)-(VI.3b)).

Thus one finds by explicit integration for the first additional potential function $\varepsilon_I(\nu)$ (G.17b):

$$\begin{aligned}\varepsilon_I(\nu) &= \frac{2\nu+2}{2^{4\nu+4}} \sum_{m,n=0}^{\infty} \frac{1}{2^{m+n}} \cdot \frac{\Gamma(4\nu+4+m+n)}{\Gamma(2\nu+3+m) \cdot \Gamma(2\nu+4+n)} \\ &\stackrel{2\nu \text{ int.}}{\implies} (2\nu+2) \cdot \varepsilon_{\text{pot}}(\nu) - \frac{1}{2\nu+1} \left(1 - \frac{1}{(2\nu)! 2^{2\nu+1}} \cdot \sum_{n=0}^{2\nu+1} \frac{1}{2^n} \cdot \frac{(2\nu+n)!}{n!} \right) .\end{aligned}\quad (\text{G.19})$$

Next the second potential function $\varepsilon_{II}(\nu)$ (G.17c) obviously splits up into two contributions where the first one is closely related to the original function $\varepsilon_{\text{pot}}(\nu)$ (G.17a) with a shift $\nu \rightarrow \nu + \frac{1}{2}$ so that this second function appears as

$$\varepsilon_{II}(\nu) = \varepsilon'_{II}(\nu) + \varepsilon''_{II}(\nu) \quad (\text{G.20a})$$

$$\varepsilon'_{II}(\nu) \doteq \int dy y^2 \frac{e_{\nu+\frac{1}{2}}(y) \cdot e_{\nu+\frac{1}{2}}(y)}{\Gamma(2\nu+2)^2} = (2\nu+2)^2 \cdot \varepsilon_{\text{pot}}(\nu + \frac{1}{2}) \quad (\text{G.20b})$$

$$\begin{aligned}\varepsilon''_{II}(\nu) &\doteq \frac{1}{2} \int dy y^2 \frac{e_{\nu}(y) \cdot e_{\nu+1}(y)}{\Gamma(2\nu+2)^2} \\ &= \frac{(\nu+1)(2\nu+3)}{2^{4\nu+5}} \sum_{m,n=0}^{\infty} \frac{1}{2^{m+n}} \cdot \frac{\Gamma(4\nu+5+m+n)}{\Gamma(2\nu+5+m) \Gamma(2\nu+3+n)} \\ &\stackrel{2\nu \text{ int.}}{\implies} (\nu+1)(2\nu+3) \left\{ \sum_{\substack{m=2\nu+1 \\ (m,n=0 \\ (m+n \geq 2)}}}^{n=2\nu+3} \frac{1}{2^{m+n-1}} \cdot \frac{(m+n-2)!}{m! n!} - \sum_{n=2}^{2\nu+1} \frac{1}{n(n-1)} - \sum_{n=2}^{2\nu+3} \frac{1}{n(n-1)} \right\} .\end{aligned}\quad (\text{G.20c})$$

A similar situation does occur also for the third potential $\varepsilon_{III}(\nu)$ (G.17d). Indeed, comparing this to the first potential $\varepsilon_I(\nu)$ (G.17b) one easily realizes that both potentials differ essentially by the shift $\nu \rightarrow \nu + \frac{1}{2}$, i. e. one finds

$$\varepsilon_{III}(\nu) = (2\nu+2)^2 \cdot \varepsilon_I(\nu + \frac{1}{2}) . \quad (\text{G.21})$$

And finally, such a shift $\nu \rightarrow \nu + 1$ of the variational parameter p is also observed in connection with the original and the fourth potentials $\varepsilon_{\text{pot}}(\nu)$ (G.17a) and $\varepsilon_{IV}(\nu)$ (G.17e) so that one arrives at the following result:

$$\varepsilon_{IV}(\nu) = (2\nu+3)^2 (2\nu+2)^2 \cdot \varepsilon_{\text{pot}}(\nu + 1) . \quad (\text{G.22})$$

The generalized potential function $\varepsilon_{\text{pot}}(\nu, p)$ (G.16) is an important object for the calculation of the positronium spectrum since it is the essential constituent of the gauge field energy $E_R^{[e]}$ (G.15). The point here is that $E_R^{[e]}$ must obey the Poisson identity (III.47); otherwise the energy functional $\tilde{\mathbb{E}}_{[\Phi]}$ (III.41) could not be reduced to its physical part $\mathbb{E}^{[IV]}$ (III.55) alone which consists solely of the kinetic and potential energy (recall here that for the approximative treatment of the anisotropic configurations in **Sect. IV** the Poisson identity is not satisfied so that the energy functional must embrace also the Poisson constraint term in addition to the kinetic and potential energy, cf. (IV.29)). Therefore it is a satisfying reinsurance to see the Poisson identity being satisfied here even for the *approximative* (!) configurations $\tilde{\Phi}_{\nu p}(y)$ (G.2) and its associated potential $\tilde{a}_{\nu p}(y)$ (G.4).

In its rescaled form, the mass equivalent $\tilde{\mathbb{M}}^{[e]}c^2$ (III.48) reads

$$\tilde{\mathbb{M}}^{[e]}c^2 = -\frac{\hbar c (2\alpha_s \beta)}{\Gamma(2\nu + 2)} \int_0^\infty dy y \tilde{a}_{\nu p}(y) \cdot \tilde{\Phi}_{\nu p}^2(y) \quad (\text{G.23})$$

with the trial amplitude $\tilde{\Phi}_{\nu p}(y)$ being given by equation (G.2) and the corresponding gauge potential $\tilde{a}_{\nu p}(y)$ by equation (G.4). Thus, inserting the latter two objects into the present mass equivalent $\tilde{\mathbb{M}}^{[e]}c^2$ (G.23) yields obviously a polynomial of fourth order with respect to the variational parameters p_0, p_1 , just as is the case with the gauge field energy $E_R^{[e]}$ (G.15)-(G.16). The Poisson identity (III.47) demands now that both fourth-order polynomials must be identical which implies the identity of the coefficients in front of the various products of the parameters p_0, p_1 .

First, the lowest-order identification ($\sim p_0^4$) lets emerge the zero-order function $\varepsilon_{\text{pot}}(\nu)$ (G.17a) in terms of the potential $a_\nu(y)$ in the following alternative way

$$\varepsilon_{\text{pot}}(\nu) = -\frac{1}{\Gamma(2\nu + 2)^2} \int dy y^{2\nu+1} e^{-y} \cdot a_\nu(y) , \quad (\text{G.24})$$

i. e. for integer 2ν

$$\varepsilon_{\text{pot}}(\nu) = \frac{1}{2\nu + 1} \left\{ 1 - \frac{1}{(2\nu + 1)! 2^{2\nu+1}} \sum_{n=0}^{2\nu} \frac{2\nu + 1 - n}{2^n} \cdot \frac{(2\nu + n)!}{n!} \right\} \quad (\text{G.25})$$

whose generalization to arbitrary ν is then given by equation (A.28).

Next, the identification of the linear terms ($\sim p_0^3 p_1$) lets emerge the first-order function $\varepsilon_I(\nu)$ (G.17b) alternatively in terms of the potential $a_\nu(y)$ as follows

$$\begin{aligned}\varepsilon_I(\nu) &= -\frac{1}{\Gamma(2\nu+2)^2} \int dy y^{2\nu+2} e^{-y} \cdot a_\nu(y) \\ &= -\frac{1}{\Gamma(2\nu+2)^2} \int dy y^{2\nu+1} e^{-y} \cdot a_{\nu+\frac{1}{2}}(y),\end{aligned}\quad (\text{G.26})$$

i. e. for integer 2ν :

$$\begin{aligned}\varepsilon_I(\nu) &= 1 - \frac{1}{(2\nu+1) \cdot (2\nu+1)!} \frac{1}{2^{2\nu+2}} \sum_{n=0}^{2\nu} \frac{2\nu+1-n}{2^n} \cdot \frac{(2\nu+1+n)!}{n!} \\ &= \frac{2\nu+2}{2\nu+1} \left\{ 1 - \frac{2\nu+1}{(2\nu+2)!} \frac{1}{2^{2\nu+1}} \sum_{n=0}^{2\nu+1} \frac{2\nu+2-n}{2^n} \cdot \frac{(2\nu+n)!}{n!} \right\},\end{aligned}\quad (\text{G.27})$$

or more generally for arbitrary ν :

$$\begin{aligned}\varepsilon_I(\nu) &= \frac{2\nu+2}{2\nu+1} \left\{ 1 - \frac{1}{\Gamma(2\nu+3) \cdot 2^{4\nu+3}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+3+n)}{\Gamma(2\nu+2+n)} \right\} \\ &= 1 - \frac{1}{\Gamma(2\nu+2) \cdot 2^{4\nu+3}} \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+3+n)}{\Gamma(2\nu+3+n)}.\end{aligned}\quad (\text{G.28})$$

Furthermore, the identification of the quadratic terms ($\sim p_0^2 \cdot p_1^2$) confirms the former splitting (G.20a) into two parts $\varepsilon''_{\text{II}}(\nu)$ and $\varepsilon'_{\text{II}}(\nu)$ with the first part $\varepsilon'_{\text{II}}(\nu)$ being given by equation (G.20b). The second part $\varepsilon''_{\text{II}}(\nu)$ is found in terms of the potential $a_\nu(y)$ as follows

$$\begin{aligned}\varepsilon''_{\text{II}}(\nu) &= -\frac{1}{2 \cdot \Gamma(2\nu+2)^2} \int dy y^{2\nu+3} e^{-y} \cdot a_\nu(y) \\ &= -\frac{1}{2 \cdot \Gamma(2\nu+2)^2} \int dy y^{2\nu+1} e^{-y} \cdot a_{\nu+1}(y),\end{aligned}\quad (\text{G.29})$$

i. e. explicitly for integer 2ν

$$\begin{aligned}\varepsilon''_{\text{II}}(\nu) &= (\nu+1) \left\{ 1 - \frac{1}{(2\nu+2)! \cdot 2^{2\nu+3}} \cdot \sum_{n=0}^{2\nu} \frac{1}{2^n} \frac{2\nu+1-n}{2\nu+1} \cdot \frac{(2\nu+2+n)!}{n!} \right\} \\ &= \frac{(\nu+1)(2\nu+3)}{2\nu+1} \left\{ 1 - \frac{1}{(2\nu)!} \frac{1}{2^{2\nu+1}} \cdot \sum_{n=0}^{2\nu+2} \frac{1}{2^n} \frac{2\nu+3-n}{2\nu+3} \cdot \frac{(2\nu+n)!}{n!} \right\}.\end{aligned}\quad (\text{G.30})$$

For arbitrary ν , this result is generalized to

$$\begin{aligned}\varepsilon''_{\text{II}}(\nu) &= \frac{(\nu+1)(2\nu+3)}{2\nu+1} \left\{ 1 - \frac{1}{\Gamma(2\nu+4) \cdot 2^{4\nu+4}} \cdot \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+4+n)}{\Gamma(2\nu+2+n)} \right\} \quad (\text{G.31}) \\ &= (\nu+1) \left\{ 1 - \frac{1}{\Gamma(2\nu+2) \cdot 2^{4\nu+4}} \cdot \sum_{n=0}^{\infty} \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+4+n)}{\Gamma(2\nu+4+n)} \right\}.\end{aligned}$$

Finally, the last two auxiliary functions $\varepsilon_{\text{III}}(\nu)$ (G.17d) and $\varepsilon_{\text{IV}}(\nu)$ (G.17e) are recovered by the identification process to undergo the former relationships (G.21)-(G.22) and therefore need not be reproduced explicitly once more. Thus the overall result is that the total potential function $\varepsilon_{\text{pot}}(\nu, p)$ is built up by only *three* “independent” auxiliary potential functions $\varepsilon_{\text{pot}}(\nu)$ (A.28), $\varepsilon_{\text{I}}(\nu)$ (G.28) and $\varepsilon''_{\text{II}}(\nu)$ (G.31). The subsequent table displays the values of these auxiliary functions on the relevant values of the variational parameter ν .

ν	$\varepsilon_{\text{pot}}(\nu)$ (A.28),(G.18),(G.25)	$\varepsilon_{\text{I}}(\nu)$ (G.19), (G.21), (G.28)	$\varepsilon_{\text{II}}(\nu)$ (G.20a)-(G.20c), (G.29)-(G.31)	$\varepsilon_{\text{III}}(\nu)$ (G.21)	$\varepsilon_{\text{IV}}(\nu)$ (G.22)
0	1/2	3/4	17/8	25/8	33/4
1/2	5/16	25/32	27/8	231/32	837/32
1	11/48	77/96	895/192	837/64	965/16
3/2	93/512	837/1024	6115/1024	10615/512	59475/512
1.7942	11410011/70398355	18307008/22197935	30171115/4469191	67286322/2579651	127537747/790294
2	193/1280	2123/2560	37371/5120	30927/1024	101997/512
5/2	793/6144	10309/12288	53081/6144	169995/4096	1290317/4096
3	1619/14336	24285/28672	572891/57344	447661/8192	480429/1024
7/2	26333/262144	447661/524288	5950665/524288	9128151/131072	87461775/131072
3.758	0.095054241197409	0.857009038635841	12.054442498170000	78.107662353796800	788.549642958726000
5.8740	0.066169154715619	0.876608961672518	17.889125526774400	166.345557346382000	2381.422474398040000
8.1307	0.050122450469590	0.890244891770568	24.190554653983300	297.684754381852000	5602.879738648750000
10.5044	0.040003065289686	0.900420995992488	30.876199420891700	477.632653223513000	11254.456630209200000
20.9538	0.021304380884411	0.924772043678155	60.694395455665500	1784.286219086780000	79307.664262054600000
35.7017	0.012897315290706	0.940258135564422	103.307086974352000	5068.138932269630000	374712.658866740000000
51.9196	0.009013462373609	0.949470915666053	150.512127748210000	10638.361918298200000	1131556.682871470000000
69.3583	0.006816023482166	0.955719638189442	201.500567239779000	18927.246550543200000	2673278.362712070000000
87.8627	0.005418519284556	0.960299247611835	255.774202228416000	30335.614989561300000	5407202.467179070000000
107.3506	0.004458053255881	0.963836463562330	313.064859152140000	45264.878166797100000	9832433.121974210000000
127.8215	0.003759305734937	0.966679154371855	373.353836428638000	64172.139638711000000	16566692.535880100000000
149.3660	0.003227635139863	0.969039351893033	436.897193397184000	87644.083923089700000	26402600.563888400000000
172.1617	0.002807948458097	0.971054276427006	504.212697547382000	116472.927171035000000	40397270.423721200000000
222.5187	0.002182090441513	0.974384926745674	653.142502031965000	194728.948425671000000	87151050.944645500000000
280.9497	0.001734286200261	0.977095438492802	826.236162746333000	310705.515336457000000	175365719.699678000000000
348.2858	0.001402947397976	0.979356411386679	1025.982804702670000	477935.192145890000000	334116453.208982000000000
422.8567	0.001158190262783	0.981230916467000	1247.450242037150000	705138.107234676000000	598116579.333488000000000
501.4654	0.000978443179650	0.982771788905577	1481.148639701370000	992496.232749923000000	997902240.046021000000000

Appendix H: *Alternative Parametrization of Trial Amplitude $\tilde{\Phi}(r)$*

The normalization condition (VI.2) for the trial amplitude $\tilde{\Phi}_b(r)$ (VI.1) reduces the parameter space \mathbb{R}^2 of the two real-valued ansatz parameters b_0, b_1 to some one-dimensional compact subspace which is topologically equivalent to the circle \mathcal{S}^1 . This entails ultimately that the energy function $E_T(\nu, p_0, p_1)$ (VI.26) must be extremalized on the half-cylinder given by the constraint (VI.2) together with the condition $-\frac{1}{2} < \nu < \infty$. However, it may be instructive to use as the underlying parameter space also a half-plane $\{-\frac{1}{2} < \nu < \infty, -\infty < p < +\infty\}$. In this sense, one parametrizes the generalized trial amplitude $\tilde{\Phi}_b(r)$ (VI.1) in the following alternative way

$$\tilde{\Phi}_b(r) = \Phi_* r^\nu (1 + br) e^{-\beta r} \quad (\text{H.1a})$$

$$\Phi_*^2(r) = \frac{2}{\pi} \frac{(2\beta)^{2\nu+2}}{\Gamma(2\nu+2)} \cdot \frac{1}{w^2(\nu, p)}, \quad (\text{H.1b})$$

where the denominator $w(\nu, p)$ in (H.1b) is given by

$$w(\nu, p) = \sqrt{1 + 4(\nu + 1) \cdot p + 2(\nu + 1)(2\nu + 3) \cdot p^2} \quad (\text{H.2})$$

and the variational parameter p is related to the original ansatz parameter b through

$$p \doteq \frac{b}{2\beta}. \quad (\text{H.3})$$

Substituting this back into the original ansatz (H.1a) for $\tilde{\Phi}_b(r)$, one arrives at the following form of the trial amplitude

$$\tilde{\Phi}_b(r) = \sqrt{\frac{2}{\pi}} \frac{2\beta}{\sqrt{\Gamma(2\nu+2)}} \cdot \frac{\tilde{\Phi}_{\nu w}(y)}{w(\nu, p)} \quad (\text{H.4a})$$

$$\tilde{\Phi}_{\nu w}(y) \doteq y^\nu (1 + py) e^{-\frac{y}{2}}. \quad (\text{H.4b})$$

Here, the original normalization condition (III.38) on $\tilde{\Phi}_b(r)$ transcribes to the present reduced amplitude $\tilde{\Phi}_{\nu w}(y)$ (H.4b) as

$$\frac{1}{\Gamma(2\nu + 2) \cdot w(\nu, p)} \int_0^\infty dy y \tilde{\Phi}_{\nu w}(y) = 1 . \quad (\text{H.5})$$

Kinetic Energy

After the reparametrization of the trial amplitude is fixed now, one can next turn to the kinetic energy E_{kin} (III.42)–(III.44) in terms of the new parameters p, w . Here, the radial kinetic energy ${}^{(r)}E_{\text{kin}}$ (III.43) emerges in terms of the new parametrization as

$${}^{(r)}E_{\text{KIN}} = \frac{e^2}{2a_B} (2\beta a_B)^2 \cdot \frac{{}^{(r)}\varepsilon_{\text{KIN}}(\nu, p)}{w^2(\nu, p)} \quad (\text{H.6})$$

with the radial kinetic function ${}^{(r)}\varepsilon_{\text{KIN}}(\nu, p)$ being defined by

$${}^{(r)}\varepsilon_{\text{KIN}}(\nu, p) = \frac{1}{\Gamma(2\nu + 2)} \int_0^\infty dy y \left[\frac{d\tilde{\Phi}_{\nu w}(y)}{dy} \right]^2 . \quad (\text{H.7})$$

The explicit calculation of this integral by use of the dimensionless trial amplitude $\tilde{\Phi}_{\nu w}(y)$ (H.4b) lets then emerge this radial kinetic function in the following form

$${}^{(r)}\varepsilon_{\text{KIN}}(\nu, p) = \frac{1}{4(2\nu + 1)} + \frac{\nu}{2\nu + 1} \cdot p + \frac{1}{2}(\nu + 1) \cdot p^2 , \quad (\text{H.8})$$

i. e. a quadratic function with respect to the additional parameter p (H.3).

Of course, the kinetic energy is an observable quantity and therefore cannot depend upon the special parametrization of the wave function $\tilde{\Phi}_b(r)$. This means that both parametrizations (VI.1)–(VI.3b) and (H.1a)–(H.5) must generate the same kinetic energy, i. e. both results (VI.5) and (H.6) for the radial type of energy must be identical

$${}^{(r)}E_{\text{kin}}(\beta; \nu, p_0, p_1) \stackrel{!}{=} {}^{(r)}E_{\text{KIN}}(\beta; \nu, p) . \quad (\text{H.9})$$

But this requirement says now that there must exist a diffeomorphism which relates the half-cylinder, being defined by the constraint (VI.2) together with $-\frac{1}{2} < \nu < \infty$, to the half-plane $\{-\infty < p < \infty; -\frac{1}{2} < \nu < \infty\}$; and this then must guarantee the identification (H.9). The desired map is specified by the following simple transformation

$$w = \frac{1}{p_0} \quad (\text{H.10a})$$

$$p = \frac{p_1}{p_0}, \quad (\text{H.10b})$$

since by this relationship both kinetic functions ${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.6)–(VI.7) and ${}^{(r)}\varepsilon_{\text{KIN}}(\nu, p)$ (H.7)–(H.8) become linked through

$${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) \Rightarrow \frac{{}^{(r)}\varepsilon_{\text{KIN}}(\nu, p)}{w^2(\nu, p)} \quad (\text{H.11})$$

so that the required numerical identity (H.9) can actually be true.

Similar arguments may also be used in order to set up the longitudinal kinetic energy ${}^{(\vartheta)}E_{\text{KIN}}(\beta; \nu, p)$ (III.44)

$$\begin{aligned} {}^{(\vartheta)}E_{\text{KIN}}(\beta; \nu, p) &\doteq \frac{\hbar^2}{2M} l_\varphi^2 \cdot \frac{\pi}{2} \int_0^\infty \frac{dr}{r} \tilde{\Phi}_b^2(r) \\ &\doteq \frac{e^2}{2a_B} (2a_B\beta)^2 l_\varphi^2 \cdot \frac{{}^{(\vartheta)}\varepsilon_{\text{KIN}}(\nu, p)}{w(\nu, p)^2}, \end{aligned} \quad (\text{H.12})$$

with the longitudinal kinetic function being found as

$${}^{(\vartheta)}\varepsilon_{\text{KIN}}(\nu, p) = \frac{1}{2\nu(2\nu+1)} + \frac{2}{2\nu+1} \cdot p + p^2. \quad (\text{H.13})$$

Of course, this kinetic function arises again also through applying the parameter transformation (H.10a)–(H.10b) to the former kinetic function ${}^{(r)}\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.9)

$${}^{(\vartheta)}\varepsilon_{\text{kin}}(\nu, p_0, p_1) \Rightarrow \frac{{}^{(\vartheta)}\varepsilon_{\text{KIN}}(\nu, p)}{w^2(\nu, p)}. \quad (\text{H.14})$$

Such a transformation must then also hold for the total kinetic function $\varepsilon_{\text{KIN}}(\nu, p)$

$$\begin{aligned} \varepsilon_{\text{KIN}}(\nu, p) &= {}^{(r)}\varepsilon_{\text{KIN}}(\nu, p) + {}^{(\vartheta)}\varepsilon_{\text{KIN}}(\nu, p) \cdot l_\varphi^2 \\ &= \frac{\nu + 2l_\varphi^2}{4\nu(2\nu+1)} + \frac{\nu + 2l_\varphi^2}{(2\nu+1)} \cdot p + \left(\frac{\nu+1}{2} + l_\varphi^2 \right) \cdot p^2, \end{aligned} \quad (\text{H.15})$$

i. e. the action of the parameter transformation (H.10a)–(H.10b) on the total kinetic function $\varepsilon_{\text{kin}}(\nu, p_0, p_1)$ (VI.11) reads

$$\varepsilon_{\text{kin}}(\nu, p_0, p_1) \Rightarrow \frac{\varepsilon_{\text{KIN}}(\nu, p)}{w^2(\nu, p)} . \quad (\text{H.16})$$

Interaction Energy

Clearly, the intrinsic consistency of the reparametrization demands that an analogous relationship must apply also to the potential energy $E_{\text{R}}^{[\text{e}]} \left(= \tilde{M}^{[\text{e}]} c^2 \right)$ (VI.12). The counterpart of this object ($E_w^{[\text{e}]}$, say) is built up by the interaction potential ${}^{[p]}A_w(r)$ as the counterpart of ${}^{[p]}A_0(r)$ in the same way as for the first parametrization, cf. (III.45), i. e.

$$E_w^{[\text{e}]} = -\frac{\hbar c}{\alpha_s} \int_0^\infty dr r^2 \cdot \left(\frac{d {}^{[p]}A_w(r)}{dr} \right)^2 . \quad (\text{H.17})$$

Here, the reparametrized potential ${}^{[p]}A_w(r)$ is the counterpart of the former ${}^{[p]}A_0(r)$ and is also the solution of the Poisson equation (III.36), albeit with regard to the reparametrized source-term (H.4a)–(H.4b)

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) {}^{[p]}A_w(r) = -\frac{\pi}{2} \alpha_s \frac{\tilde{\Phi}_b^2(r)}{r} , \quad (\text{H.18})$$

or rewritten in dimensionless form (${}^{[p]}A_w(r) \doteq 2\beta\alpha_s \cdot \tilde{a}_{\nu w}(y)$)

$$\Delta_y \tilde{a}_{\nu w}(y) = -\frac{1}{\Gamma(2\nu + 2) \cdot w^2(\nu, p)} \cdot \frac{\tilde{\Phi}_{\nu w}^2(y)}{y} \quad (\text{H.19})$$

where the dimensionless form $\tilde{\Phi}_{\nu w}(y)$ is already displayed by equation (H.4b). This special form of the Poisson equation suggests again to compose its solution $\tilde{a}_{\nu w}(y)$ from the more elementary potentials $a_\nu(y)$ (G.13a) as the solutions of the simplified Poisson equation (G.5), i. e. we put again

$$\tilde{a}_{\nu w}(y) = -\frac{a_\nu(y) + 2p \cdot a_{\nu+\frac{1}{2}}(y) + p^2 \cdot a_{\nu+1}(y)}{\Gamma(2\nu + 2) \cdot w^2(\nu, p)} \quad (\text{H.20})$$

where the elementary potentials $a_\nu(y)$ obey the simplified Poisson equation (G.5) and therefore are given by equation (G.11) for integer 2ν , and by equation (G.13a) for arbitrary ν (but $\nu > -\frac{1}{2}$). Substituting this solution $\tilde{a}_{\nu w}(y)$ (H.20) back into the electrostatic field energy $E_w^{[e]}$ (H.17) (or equivalently into its mass equivalent) lets then appear the latter objects in the following form

$$E_w^{[e]} = \tilde{\mathbb{M}}_w^{[e]} c^2 = -\frac{e^2}{a_B} (2\beta a_B) \cdot \frac{\varepsilon_{\text{POT}}(\nu, p)}{w^4(\nu, p)}, \quad (\text{H.21})$$

with the alternative potential function $\varepsilon_{\text{POT}}(\nu, p)$ being found as

$$\varepsilon_{\text{POT}}(\nu, p) = \varepsilon_{\text{pot}}(\nu) + 4p \cdot \varepsilon_I(\nu) + 4p^2 \cdot \varepsilon_{II}(\nu) + 4p^3 \cdot \varepsilon_{III}(\nu) + p^4 \cdot \varepsilon_{IV}(\nu). \quad (\text{H.22})$$

The crucial point is here that this alternative form of the potential function just guarantees the numerical identity of both electrostatic field energies $E_R^{[e]}$ (G.15) and $E_w^{[e]}$ (H.21):

$$E_R^{[e]} \equiv E_w^{[e]} \quad (\text{H.23a})$$

$$\left(\tilde{\mathbb{M}}^{[e]} c^2 \equiv \tilde{\mathbb{M}}_w^{[e]} c^2 \right). \quad (\text{H.23b})$$

Indeed, applying the parameter transformation (H.10a)–(H.10b) to the original potential function $\varepsilon_{\text{pot}}(\nu, p_0, p_1)$ (VI.13) yields the transition

$$\varepsilon_{\text{pot}}(\nu, p_0, p_1) \Rightarrow \frac{\varepsilon_{\text{POT}}(\nu, p)}{w^4(\nu, p)} \quad (\text{H.24})$$

and this is just what validates the claimed numerical identity (H.23a).

Finally, the value of the total energy functional $\mathbb{E}^{[\text{IV}]}$ on the selected trial configurations appears now again in the form of the following energy function

$$E_T(\beta, \nu, p) = 2E_{\text{KIN}}(\beta, \nu, p) + E_w^{[e]}(\beta, \nu, p) \quad (\text{H.25})$$

$$= \frac{e^2}{a_B} \left\{ (2\beta a_B)^2 \cdot \frac{\varepsilon_{\text{KIN}}(\nu, p)}{w^2(\nu, p)} - (2\beta a_B) \cdot \frac{\varepsilon_{\text{POT}}(\nu, p)}{w^4(\nu, p)} \right\}$$

with the kinetic function $\varepsilon_{\text{KIN}}(\nu, p)$ being specified by equation (H.15) and the potential function $\varepsilon_{\text{POT}}(\nu, p)$ by (H.22).

Extremal Configurations

In order to determine the extremal values of the energy functional $\mathbb{E}^{[IV]}$ on the selected trial functions, one has again to determine the local minima of the total energy $E_T(\beta, \nu, p)$ (H.25) for any l_ϕ . This is equivalent to looking for the minima of the reduced energy function $\mathbb{E}_T(\nu, p)$

$$\mathbb{E}_T(\nu, p) = -\frac{e^2}{4a_B} \cdot S_P(\nu, p) \quad (\text{H.26a})$$

$$S_P(\nu, p) = \frac{\varepsilon_{\text{POT}}^2(\nu, p)}{\varepsilon_{\text{KIN}}(\nu, p) \cdot w^6(\nu, p)} . \quad (\text{H.26b})$$

The local maxima of the spectral function S_P (H.26b) determine now the binding energies as the local minima of the total energy $\mathbb{E}_T(\nu, p)$ (H.26a).

For a brief demonstration of the present approximation method, one may consider the groundstate ($l_\phi = 0 \Rightarrow n_P = 1$). Obviously, the roughest approximation is specified by putting both variational parameters ν and p to zero. For this situation, the kinetic function ε_{KIN} (H.15) becomes simplified to

$$\varepsilon_{\text{KIN}}(0, 0) = \frac{1}{4} . \quad (\text{H.27})$$

Furthermore, the potential function ε_{POT} (H.22) becomes reduced to

$$\varepsilon_{\text{POT}}(0, 0) = \varepsilon_{\text{pot}}(0) = \frac{1}{2} , \quad (\text{H.28})$$

and the function $w(\nu, p)$ (H.2) collapses to unity

$$w(0, 0) = 1 . \quad (\text{H.29})$$

Consequently, the spectral function $S_P(\nu, p)$ (H.26b) adopts the unity

$$S_P(0, 0) = 1 , \quad (\text{H.30})$$

and therefore the positronium groundstate energy $\mathbb{E}_T(\nu, p)$ (H.26a) is found in this roughest approximation as

$$\mathbb{E}_T(0, 0) = -\frac{e^2}{4a_B} \simeq -6,8029 \dots \text{ [eV]} . \quad (\text{H.31})$$

This is *exactly* the value predicted by the conventional theory, cf. (I.4); but within the present RST framework it appears as an *approximation!* Therefore one expects that in the next higher approximation the corresponding RST prediction for the groundstate must yield some lower energy value; and indeed, putting p to zero and thus admitting only two variational parameters (i. e. β, ν) yields a groundstate prediction of $-7,23055\dots$ [eV] in place of the conventional prediction (H.31), see first line of **table 1** on p. 44.

Alternatively, one could have taken as the next higher approximation also $\nu = 0$ and leaving p as the second variational parameter. In this case, the kinetic function ε_{KIN} (H.15) is simplified for the groundstate ($l_\varphi = 0$) to

$$\varepsilon_{\text{KIN}}(0, p) = \frac{1}{4} + \frac{1}{2}p^2 \quad (\text{H.32})$$

and, furthermore, the potential function ε_{POT} (H.22) becomes

$$\varepsilon_{\text{POT}}(0, p) = \varepsilon_{\text{pot}}(0) + 4p \cdot \varepsilon_{\text{I}}(0) + 4p^2 \cdot \varepsilon_{\text{II}}(0) + 4p^3 \cdot \varepsilon_{\text{III}}(0) + p^4 \cdot \varepsilon_{\text{IV}}(0) , \quad (\text{H.33})$$

i. e. by use of the table in **App. G**

$$\varepsilon_{\text{POT}}(0, p) = \frac{1}{2} + 3p + \frac{17}{2}p^2 + \frac{25}{2}p^3 + \frac{33}{4}p^4 . \quad (\text{H.34})$$

This together with $w(0, p)$ (H.2) builds up the spectral function $S_{\mathcal{P}}$ (H.26b) to the following form

$$S_{\mathcal{P}}(0, p) \doteq S_{\mathcal{P}}^{[0]}(p) = \frac{\{1 + 6p + 17p^2 + 25p^3 + \frac{33}{2}p^4\}^2}{(1 + 2p^2) \cdot [1 + 4p + 6p^2]^3} . \quad (\text{H.35})$$

The present alternative parametrization serves as a technical consistency check for our numerical program of approximately determining the positronium binding energies $E_{\mathcal{P}}^{[n]} = E_{\text{T}}(\nu_*^{[n]}, p_n)$; and it is very satisfying to see the positronium energies E_{1a} up to E_{1d} (VI.40a)-(VI.40b) of the compact parametrization (VI.36a)-(VI.36b) emerging also in the alternative open parametrization (H.10a)-(H.10b), see the **Fig. H.I** below.

Concerning now the excited states, one has to relax the adhoc postulate $\nu = 0$ of the simplified groundstate treatment and thus one has to admit any real value of $\nu (>$

$-\frac{1}{2}$). This means that one has to look for the maximum of the spectral function $S_\phi(\nu, p)$ (H.26b) as a function of the two variables ν and p . This may be done by means of an appropriate computer program, for the first excited state ($n_\phi = 2 \Leftrightarrow l_\phi = 1$) one finds the maximum $S_\phi^{[2]}(*) = 0, 229683 \dots$ of the spectral function $S_\phi(\nu, p)$ (H.26b) at the equilibrium point

$$\nu_*^{[2]} = 1, 258290 \dots \quad (\text{H.36a})$$

$$p_*^{[2]} = 0, 677982 \dots \quad (\text{H.36b})$$

Thus, the energy $E_\phi^{[2]}$ of the first excited state is obtained in the present (spherically symmetric) approximation step as

$$\begin{aligned} E_\phi^{[2]} &= -\frac{e^2}{4a_B} \cdot S_\phi^{[2]}(x) \simeq -6, 8029 \cdot 0, 2296 \text{ [eV]} \\ &\simeq -1, 56194 \text{ [eV]} \end{aligned} \quad (\text{H.37})$$

Comparing this to the corresponding first-order approximation (of the spherically symmetric kind) $\mathbb{E}_T(\nu_*^{[2]})$ (see second line of table 1 on p.(?))

$$\mathbb{E}_T(\nu_*^{[2]}) = -1, 55087 \text{ [eV]} \quad (\text{H.38})$$

one observes an improvement (of the deviation from the conventional result $E_{\text{conv}}^{(2)}$ (I.4)) from 8,8% (last column of table 1) to presently 8,2%:

$$\frac{E_{\text{conv}}^{[2]} - \mathbb{E}_p^{[2]}}{E_{\text{conv}}^{[2]}} = \frac{1, 70058 - 1, 56194}{1, 70058} \% = 8, 2\% \quad (\text{H.39})$$

This is a relatively small improvement in view of those improvements due to the regard of anisotropy which yielded a corresponding improvement from 8,8% to 3,1% (see first line of table 2 on p.(x)). Similar magnitudes of improvement are also found for the higher excited states (see table 3 on p.(x)). Thus the conclusion is that the first-order anisotropy corrections (**Sect.V**) are much more important than the second-order corrections of the spherically symmetric kind.

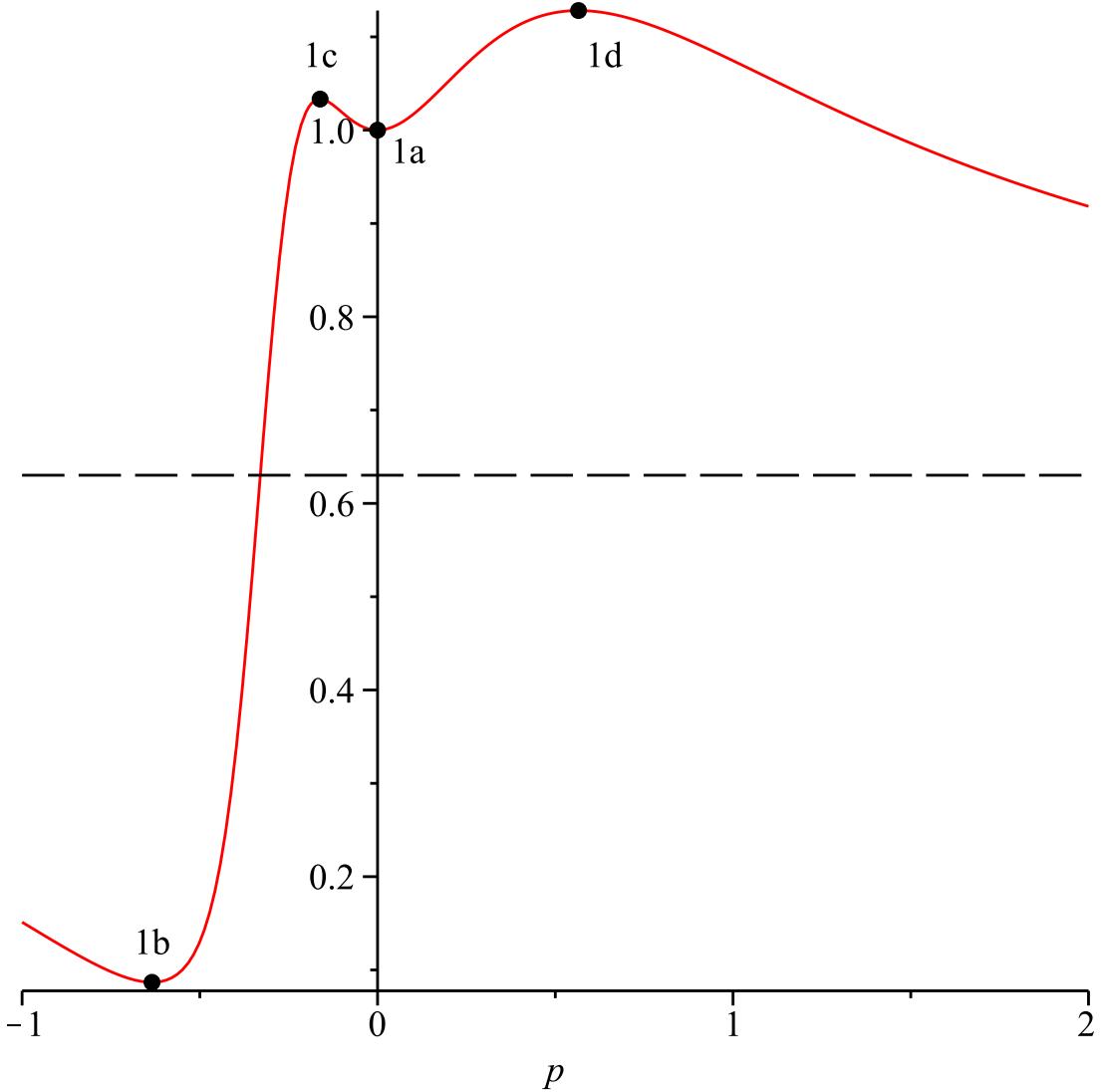


Fig. H.I Spectral Function $S_\varphi^{[0]}(p)$

The spectral function $S_\varphi^{[0]}(p)$ (H.35) possesses two relative maxima at $p_{1c} = -0, 161651\dots$ and $p_{1d} = 0, 565338\dots$ with the corresponding maximal values $S_\varphi^{[0]}|_{1c} = 1, 033319\dots$ and $S_\varphi^{[0]}|_{1d} = 1, 128194\dots$ which by means of (H.26a) yields the two energy minima E_{1c} (VI.40a) and E_{1d} (VI.40b). The two relative *minima* 1a and 1b of $S_\varphi^{[0]}(p)$ are found at $p_{1a} = 0$ and $p_{1b} = -0, 634469\dots$ which yield the two energy maxima E_{1a} (VI.39a) and E_{1b} (VI.39b) of the angular parameterization in **Sect.VI.3**. Both asymptotic values

of $S_\varphi^{[0]}(p)$ for infinity ($p \rightarrow \pm\infty$) do agree

$$\lim_{p \rightarrow \pm\infty} S_\varphi^{[0]}(p) = \frac{121}{192} \simeq 0,6302\dots \quad (\text{H.40})$$

so that the real line ($-\infty < p < +\infty$) of the present parameterization may be compactified to the circle S^1 ($0 \leq \alpha \leq 2\pi$) of the first parameterization in **Sect.(VI.3)**.

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